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FLAME SPEED DATA REDUCTION  
AND CORRELATION USING A DIGITAL COMPUTER

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Flight Accessories Laboratory  
Aeronautical Systems Division  
Air Force Systems Command  
Wright-Patterson Air Force Base, Ohio

Project No. 6075 Task No. 607505



(Prepared under Contract No. AF 33(657)-7617  
by Monsanto Research Corporation, Dayton,  
Ohio; G. H. Ringrose, D. R. Miller, A. C.  
Pauls and G. B. Skinner, authors)

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## FOREWORD

This report describes work performed under Contracts AF 33(616)-7757 and AF 33(657)-7617, "A Research Program for Understanding the Mechanisms of Flame Inhibition," and AF 33(616)-7458, "Fire-Resistant High Temperature Hydraulic Fluids." The former contract was initiated under Project No. 6075, "Flight Vehicle Hazard Protection," Task No. 607505, "A Research Program for Understanding the Mechanisms of Flame Inhibition." The latter was initiated under Project No. 7340, "Non-Metallic and Composite Materials," Task No. 734008, "Power Transmission, Heat Transfer Fluids, and Other Forms of Energy Transfer Fluids."

The contracts were performed at the Dayton Laboratory of Monsanto Research Corporation. The first two contracts were sponsored by the Flight Accessories Laboratory, Aeronautical Systems Division, Wright-Patterson Air Force Base, Ohio with Mr. Benito P. Botteri serving as project engineer. The third contract was sponsored by the Directorate of Materials Processes, Aeronautical Systems Division, Wright-Patterson Air Force Base, Ohio with Mr. Harold Adams as project engineer.

For Monsanto, the computer program was written by Dr. G. H. Ringrose of Monsanto Research Corporation and Dr. D. R. Miller and Dr. A. C. Pauls of Monsanto Chemical Company. Dr. G. B. Skinner served as project leader.

The authors are indebted to Dr. W. C. Hammann of Monsanto Chemical Company for the hand calculations that led to the adoption of the general mathematical approach. This contribution and the many helpful suggestions made by numerous people are acknowledged with gratitude. Particular assistance was given by Mr. D. J. Kaufman, also of Monsanto Chemical Company, who was instrumental in trouble shooting and expediting the machine solutions.

The routines were originally programmed and run on the IBM 704 computer in the Research and Engineering Division of Monsanto Chemical Company, St. Louis. Later the programs were adapted for solution by an IBM 7090, at the Aeronautical Systems Division, Wright-Patterson AFB, Ohio.

## ABSTRACT

Two digital computer routines were developed to process flame speed data resulting from the burning of compounds in air and oxygen, and to correlate particular structural configuration with flame speed.

In both routines a high degree of flexibility has been incorporated to assure efficient utilization under several foreseeable circumstances.

The first routine, FSC, processes the raw experimental data to obtain flame speeds, equivalence ratios, and the equivalence ratio at the maximum flame speed. This information is stored on a master magnetic tape for subsequent calculations.

The second routine, FSR, permits selection of specific data groups from the master tape for analysis. A linear model was chosen for the correlation.

This technical documentary report has been reviewed and is approved.

*W.C. Savage*  
WILLIAM C. SAVAGE  
Chief, Environmental Branch  
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## FLAME SPEED DATA REDUCTION AND CORRELATION USING A DIGITAL COMPUTER

### I. INTRODUCTION

Two Air Force-supported programs at this laboratory concern the relative rates of combustion of a number of chemical compounds. One program AF 33(616)-74587 deals with the synthesis of potential high temperature hydraulic fluids and the other AF 33(616)-76177 with increasing our understanding of the mechanisms of flame inhibition, the ultimate objective being the development of agents for extinguishing propellant fires.

Searches for effective fire-resistant fluids or propellant fire extinguishants would be systematized and expedited if a general method for characterizing, measuring, and predicting combustibility were at hand. Unfortunately, most flammability tests and specifications in use are so application-oriented or otherwise restricted as to be of only limited value for general use. A measure of the intrinsic ability of a material to support or inhibit combustion, as free as possible from influences peculiar to the testing procedure, is the first requisite. Given such a measure, there is then the possibility of relating combustibility to the molecular structures of materials tested and of predicting therefrom the combustibility of untested candidates.

This report describes computation routines designed to support the above approach. Flame speed - a state property of a combustible gas mixture - is the intrinsic measure of combustibility selected for use in characterization, correlation, and prediction. Earlier work, although limited to pure hydrocarbons burned in air, tends to confirm the approach adopted here.

The routines are programmed in the FORTRAN II language for IBM 7090 solution.

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## II. THEORETICAL ASPECTS

Theoretical flame speed is commonly defined as the subsonic rate of perpendicular propagation of an infinite plane flame front through the quiescent combustible gas. External forces (for example, gravitational or magnetic fields) are presumed absent or insignificant, and the flame-induced flow is assumed to be laminar and one-dimensional.

When defined in this idealized manner, flame speed is a function only of the initial temperature, pressure, and composition of the combustible gas. It is thus an intensive state property of the gas, just as are density, enthalpy, viscosity, refractive index, and the like. Moreover, flame speed is a transport property dependent upon the rates of energy, momentum, mass, and chemical exchange accompanying combustion.

Prediction of flame speed from gas temperature, pressure, and composition is a long-standing goal of combustion research. A reasonably general and accurate method would be extremely useful in solving a range of practical and theoretical problems. Combustor and propulsion system design may be cited, in addition to the materials search problems underwriting the work of this report.

In principle, flame speeds can be predicted theoretically. Simultaneous solution of the differential equations of change is possible when all important physical-chemical properties (e.g., heats of reaction, reaction rate constants, density, diffusivities, emissivity, etc.) are known. Unfortunately, many of these properties are not yet known. Combustion reaction mechanisms are normally quite complex and are consequently poorly understood. Much remains to be done, even in the identification of intermediate chemical species.

While theory is of little practical utility, empirical correlations offer considerable promise. Hibbard and Pinkel (Ref. 1) achieved a good correlation of maximum flame speed of 37 hydrocarbons (mixed with air) versus the concentrations of the various C-H bond types present. The relation used was of the form

$$u_{\max} = \sum_j b_j (c_j)_{\max} \quad (1)$$

The concentration  $(c_j)_{\max}$  of the  $j$  type bond is determined at the fuel-to-oxidizer ratio which yields the maximum flame velocity  $u_{\max}$  and the corresponding influence coefficient for this bond is designated  $b_j$ . The average per cent deviation

between the measured and predicted maximum flame speeds was about 2% for the 37 hydrocarbons correlated.

The approach of Hibbard and Pinkel was extended by Hammann and Blake (Ref. 2) in calculation of flame speed coefficients of the various bond types in fuels containing oxygen, nitrogen, sulphur, boron, and silicon in addition to carbon and hydrogen. Their correlations were based upon data obtained experimentally by burning 142 model compounds and upon data reported by Gibbs and Calcote (Ref. 3). Several modifications of the correlation model, Equation 1, were tested and Equation 1A was found to provide the most acceptable correlation.

$$\frac{u_{\max}}{(c_f)_{\max}} = \sum_j b_j n_j \quad (1A)$$

The number of  $j$ -type contributors occurring in each molecule of fuel is designated  $n_j$ .

While the agreement between the predicted and measured flame speeds was not as good as for hydrocarbons alone, the results convincingly supported the general utility of the linear correlation technique. The computer routines described in this report were used by Hammann and Blake.

#### DEFINITIONS

The following terms are used frequently throughout the report:

Contributor A countable structural feature of a fuel molecule (e.g., each hydrogen bonded to a primary carbon in ethane,  $\text{HC}-\overset{\text{H}}{\underset{\text{H}}{\text{CH}}}$ , could be classed as a contributor).

Contributor number  $j$  An identifying code number which is assigned to each defined contributor (e.g., the primary-H contributor was assigned the code number 37).

Contributor count  $n_j$  (or  $n_{ij}$ ) The number of  $j$ -type contributors contained in a molecule of fuel (or in a molecule of the  $i$ th fuel) (e.g., the contributor count of the contributor primary-H in the fuel ethane would be 6).

Fuel A material that forms a combustible mixture when mixed with an oxidant. Included are impurities, additives, and all compounds not included in the gaseous oxidant. For totalling the contributor count for mixed or composite fuels,

it is assumed that the over-all fuel has additive properties of the compounds present. For example, if  $z_i$  is the mole fraction of compound  $i$  in the fuel, and  $n_{ij}$  is the count for contributor  $j$ , then

$$n_j = z_1 n_{1j} + z_2 n_{2j} + \dots$$

Oxidant The portion of the combustible mixture which includes the oxygen and inert gases but excludes the fuel.

Equivalence Ratio The actual fuel-to-oxygen ratio divided by the fuel-to-oxygen ratio stoichiometrically required for complete combustion of the fuel oxidizer. This is a measure of the richness or leanness of the flame.

Standard Error Synonymous with the statistical quantity "standard deviation."

Data Group A unit of data pertaining to a single fuel-oxidant combination burned at various equivalence ratios but otherwise under identical conditions. The components of a data group in the order in which they are stored by the computer on master tape 6 are:

- (a) Serial Number Assigned sequentially by the computer in order of tape location.
- (b) Fuel Name Alphabetic and/or numeric representation of the fuel, e.g., (n-Pentene-2). A maximum of 12 characters (including blanks) is permitted.
- (c) Fuel Numbers Code numbers which are used to classify the types of fuel.
  - (1) Fuel Class Number General fuel type (e.g., 01-organic aliphatic; 02-organic aromatic, 00-inorganic).
  - (2) Fuel Group Number Denotes subclassification of fuel type (e.g., 06-saturated cyclic compound).
  - (3) Fuel Member Number An arbitrary code number, used to indicate sequence of experimental analysis of a particular group.
- Thus for the fuel cyclopropane the fuel number is 010601.
- (d) Data Source Number Designates the source of the data (e.g., 01-literature-, 02-experimental).

- (e) Experimental Conditions Number A code to distinguish data taken under different experimental conditions, such as temperature, pressure, per cent oxygen in oxidant, etc.
- (f) Flame speed at unity equivalence ratio,  $u_{stoc}$  (cm/sec).
- (g) Maximum flame speed,  $u_{max}$  (cm/sec).
- (h) Fuel concentration at unity equivalence ratio,  $(c_f)_{stoc}$  (molecules/cc).
- (i) Fuel concentration at the conditions of maximum flame speed  $(c_f)_{max}$  (molecules/cc).
- (j) Equivalence ratio at the maximum flame speed,  $\phi_{max}$
- (k) Number of different defined (i.e., coded) contributors in the fuel molecule.
- (l) List of the contributor code numbers with their respective counts for the fuel considered.

### III. DESCRIPTIVE OUTLINE OF THE CALCULATIONS

An analysis of the computations required to reduce the experimental data and perform the regression analyses led to the separation of the problem into two sections. The first section processes the raw experimental data and calculates the flame speeds, concentrations, and equivalence ratios. These quantities are then stored on a master reel of magnetic tape. The second section, namely, the flame speed regression section, uses this reel of magnetic tape as its input data. From these data, the regression coefficients of the flame speeds and other dependent variables are determined.

Corresponding to each of these sections is a Fortran routine that is described in detail in a later section. A general discussion of these routines follows.

#### DATA REDUCTION (Routine FSC)

The data reduction routine calculates the flame speed and related quantities from the raw data, tests these quantities for inconsistencies, and prepares or corrects the master reel of magnetic tape with acceptable data.

Flame Speed The calculations are based upon the conical (Bunsen) burner method for flame speed determination. Measured flows of the several components of the mixture are passed in laminar flow through a burner tube at a controlled temperature and pressure. A roughly conical flame front is stabilized at the mouth of the tube.

The large density gradient in the gas stream at the flame front permits the use of schlieren photographic techniques to record the flame profile. It is assumed that the flame is symmetrical about its vertical axis. Figure 1 is schlieren photograph of a typical flame cone.

The flame speed is determined by dividing the total volumetric gas flow rate by the area of the flame front. Since the flame cone photographed is seldom a "right circular cone," its surface area must be determined from measurements at several intermediate points. To do so, the diameter is measured at several heights of the cone as illustrated in Figure 2. The surface area between any two of these diameter measurements is assumed to be that of a frustum of a right circular cone. The sum of the surface areas of these frustra gives a fairly accurate value of the true flame front area. Actually, the local flame speed is slightly above the average at the cone tip

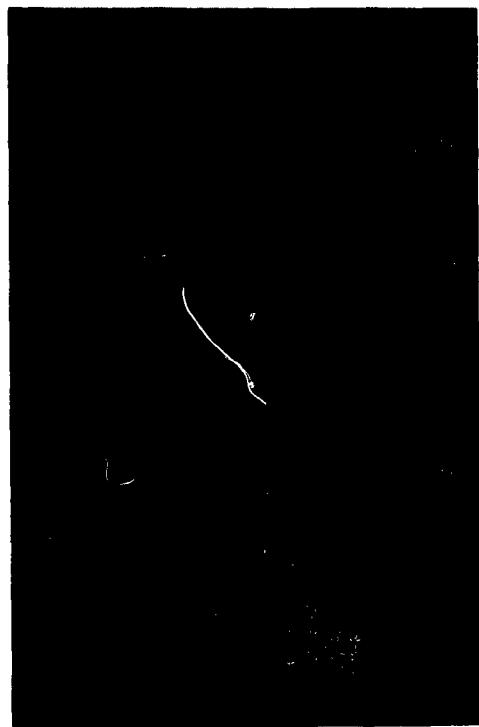


Fig. 1 Schlieren Photograph of a Flame Cone

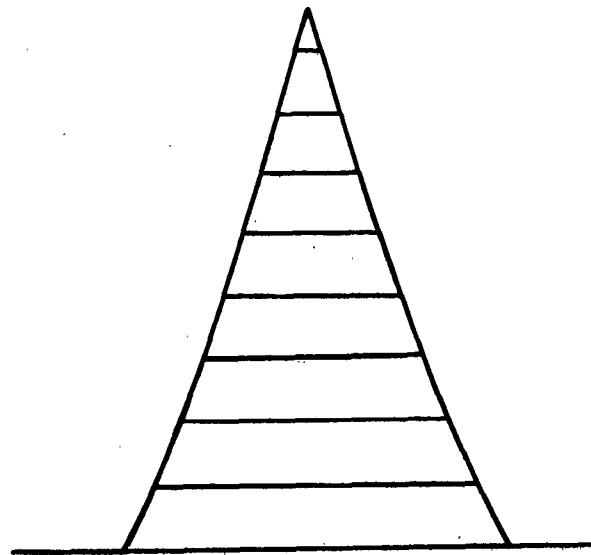


Fig. 2 Diagram of Flame Cone Profile

and slightly below the average at the base. Therefore, the calculated flame speed must be considered an average value only. Evidence has shown that there is a slight dependence of flame speed on the total volumetric flow rate of the gases, the burner part geometry, and the burner part temperature. Slight influences are also made by the method used to define the cone area (i.e., schlieren shadow, or radiant photography). However, by standardizing on one of the techniques, this variable can be eliminated.

Valid Data Tests Once a series of flame speeds has been obtained, it is necessary to determine the conditions for maximum flame speed (since the correlations proposed are based on conditions at the maximum flame speed). This is accomplished by fitting an empirical curve of flame speed vs. equivalence ratio ( $\phi$  vs.  $\phi$ ) to the data and solving the equation for the maximum. The flame speed at stoichiometric conditions ( $\phi = 1$ ) is also determined.

If a maximum flame speed lies within the data range the data are acceptable for further tests. If no maximum or a minimum is found within the data range, the data are not acceptable.

Storage on Magnetic Tape Data groups termed acceptable are stored on a master reel of magnetic tape for use by the regression routine.

Options The computational routine contains several options depending upon the form of the input data. These options permit sections of the computational procedure to be omitted. For example, a set of flame speed vs. equivalence ratio data available from previous calculations could be entered directly into the sequence, and the original raw data calculations would be by-passed. These options are detailed in Section VI.

#### FLAME SPEED REGRESSION (Routine FSC)

A multiple linear regression model similar to that used by Hibbard and Pinkel (Ref. 1)(but including a constant term) was selected:

$$y = b_0 + \sum_j b_j n_j \quad (2)$$

Independent Variables In equation (2) the independent variables were chosen to be the contributor counts rather than the contributor concentration. This simplifies the prediction and data handling, and adds flexibility by making the "independent" variables more independent. This is true because the

contributor concentrations depend upon the mixture temperature, pressure, equivalence ratio, and oxidant composition, as well as upon fuel composition. A simple relation exists between the contributor counts and concentration, as shown in Equation 3:

$$c_j = n_j c_j \text{ molecules/cc} \quad (3)$$

where  $c_f$  is the concentration of fuel in the combustible mixture. Multiplying Equation 2 by  $c_f$  gives the equivalent of the Hibbard-Pinkel model ( $b_0 = 0$ ).

Dependent Variables For the reasons mentioned above, the dependent variable  $y$  would be set equal to  $u_{\max}/(c_f)_{\max}$  when the coefficients comparable to those published by Hibbard and Pinkel are wanted. However, this is not the only dependent variable of possible interest. In predictions of maximum flame speed, for example, it is necessary to predict fuel concentration (or fuel-oxidant ratio, or equivalence ratio) at maximum flame speed. This is most readily done by correlating fuel concentration (etc.) at maximum flame speed against contributor counts. Correlations at stoichiometric fuel-oxidant ratio may be equally interesting. To emphasize that such other dependent variables can be handled with equal facility, the indefinite dependent variable  $y$  is used.

Coefficients With the emphasis so far given to fuel composition, it is appropriate to recall that calculated  $b_j$ 's are not constants. Values will depend on several or all of the following (depending on the definition of  $y$ ):

1. initial mixture temperature
2. initial mixture pressure
3. some specification of fuel-oxidant ratio
4. oxidant composition
5. contributor definitions
6. dependent variable definition

The above list includes the primary state properties. Since experimental flame speeds (distinguished from theoretical flame speeds) are always obtained under conditions differing from the ideal, values of  $b_j$  will be related to:

7. experimental conditions (oxidant composition, temperature, pressure, etc.)
8. source of data (laboratory, technique, journal reference, etc.)

All listed factors should be considered when sets of coefficients are compared.

Block Regressions Obtaining a full set of coefficients is basically a stepwise trial-and-error process. The trial-and-error enters in the definition of contributors (i.e., independent variables). Since it is not known at the outset which structural features will give the best correlations, it is necessary to accommodate definition of new contributors as the analysis progresses. In addition, it is desirable and most efficient to calculate certain coefficients using only a particular class of fuels. C-H bond coefficients, for example, are most readily and accurately determined from flame speed data on hydrocarbons. If accurately determined, a coefficient should be applicable unchanged in later regressions.

The above considerations indicated that a "block regression" procedure (certain coefficients held constant) would be most advantageous. This procedure may be expressed mathematically by Equation 4:

$$y - \sum_s b_s n_s = b_0 + \sum_u b_u n_u \quad (4)$$

The  $b_s$  coefficients represent those whose values are known, and are termed the "prespecified coefficients." The  $b_0$  and  $b_u$  coefficients are those to be determined by the regression analysis. The constant term  $b_0$  may be either calculated or prespecified as zero.

Block Selection Criteria All of the data groups that are acceptable for regression analysis are stored on a single master reel of magnetic tape. Seven different accept-reject tests are available for selection of these data. The selecting criteria comprise (1) data group serial number, (2) fuel class number, (3) fuel class-group number, (4) fuel member number, (5) data source number, (6) experimental conditions number, and (7) fuel contributor content.

For flexibility, these tests may be ignored, or applied singly or in any combination. The tests are described in detail in the following section.

#### IV. MATHEMATICAL OUTLINE OF THE CALCULATIONS

##### FLAME SPEED DATA REDUCTION CALCULATIONS (Routine FSC)

Functions Performed The functions performed by Routine FSC may be classed in five groupings. The portions of the computer program used in each function are enclosed in parentheses.

###### Function 1 (Subroutines EXPD 1 or EXPD 3)

Given: (a) Combustion mixture, temperature and pressure  
(b) Fuel stoichiometric oxygen demand  
(c) Mole fraction of  $O_2$  in oxidant  
(d) Molar volume of fuel  
(e) Volumetric flow rate of oxidant  
(f) Flame envelope dimensions

Calculate: (a) Volumetric flow rate of mixture  
(b) Area of flame envelope  
(c) Flame speed  
(d) Equivalence ratio

###### (a) Volumetric flow rate of the mixture, $q_m$

$$w_x = q_x^*/22,414 \quad \text{g-moles/sec} \quad (5)$$

$$w_f = q_f/v_f \quad \text{g-moles/sec} \quad (6)$$

$w_f$  and  $w_x$  are the molar flow rates of the fuel and oxidizer and  $q_f$  and  $q_x^*$  are the volumetric flow rates in cc/sec (the latter at S.T.P.).  $v_f$  is the molar volume of the fuel and must be based on the same fuel density as  $q_f$ .

$$v_m = 62,366(t_m + 273.15)/P_m \quad \text{cc/g-mole} \quad (7)$$

where  $v_m$  is the molar volume of the mixture and  $t_m$  ( $^{\circ}\text{C}$ ) and  $P_m$  (atm.) are the temperature and pressure of the mixture.

$$\text{Therefore: } q_m = (w_x + w_f)v_m \quad \text{cc/sec} \quad (8)$$

(b) Area of flame envelope, A

The increment of surface area  $\Delta A_i$  between any two heights  $h_i$  and  $h_{i-1}$  is given by

$$\Delta A_i = \pi \left( \frac{D_{i-1} + D_i}{2} \right) \sqrt{(h_i - h_{i-1})^2 + \left( \frac{D_{i-1} - D_i}{2} \right)^2} \text{ cm}^2 \quad (9)$$

where  $D_i$  is the measured diameter at the upper height and  $D_{i-1}$  is that at the lower height. The total surface area of the flame is calculated by summing these increments over the whole height

$$A = \sum_{i=1}^n \Delta A_i \text{ cm}^2 \quad (10)$$

(c) Flame speed, u

Once the total flame area has been determined, flame speed can be easily calculated:

$$u = q_m/A \quad (11)$$

(d) Equivalence ratio,  $\phi$

From its definition as the actual fuel-to-oxygen ratio divided by the stoichiometric fuel-to-oxygen ratio, the equivalence ratio is calculated:

$$\phi = (w_f/w_o)/(w_f/w_{ost}) \quad (12)$$

where  $w_o$  is the molar flow rate of oxygen used in the experiment and  $w_{ost}$  is that rate required for complete reaction.

$$\text{But } w_o = w_x z_{ox} \text{ g-moles/sec} \quad (13)$$

$$\text{and } w_{ost} = w_f r_{st}/2 \text{ g-moles/sec} \quad (14)$$

where  $z_{ox}$  is the mole fraction of oxygen in the oxidant and where  $r_{st}$  is the number of atoms of oxygen required to completely oxidize one molecule of fuel.

$$\text{Therefore } \phi = w_f r_{st}/2 w_x z_{ox} \quad (15)$$

### Function 2 (Subroutine MAXM)

Given: A series of experimental values of flame speed vs. equivalence ratio. (The flow rates are the only controllable variables.)

Calculate: (a) Maximum flame speed  
(b) Flame speed at stoichiometric conditions  
(c) Equivalence ratio at maximum flame speed

#### (a) Maximum flame speed, $u_{max}$

Past work has shown that curves of  $u$  vs.  $\phi$  generally are concave from below with a maximum in the vicinity of  $\phi=1$ . Figure 3 is an example of such a curve.

Many of the curves are fairly symmetrical in the vicinity of the peak and are nearly parabolic in shape. Others are fairly asymmetrical and are better approximated by a higher order power series. To find the peak of a given series of measured values of  $u$  vs.  $\phi$ , the data are fitted with an equation of the form

$$u = \sum_{r=1}^R a_r \phi^{r-1} \quad \text{cm/sec} \quad (16)$$

The method of calculating the "a" coefficients depends upon the number of points available,  $N$ . If  $N = 4$ , a perfect cubic fit ( $R = 4$ ) is obtained by solution of the simultaneous equations

$$u_n = \sum_{r=1}^R a_r \phi_n^{r-1} \quad n = 1, \dots, R \quad (17)$$

If  $N > 4$ , a least square cubic fit ( $R = 4$ ) is obtained by the solution of the "normal regression equations."

$$\sum_{n=1}^N u_n \phi_n^{r-1} = \sum_{q=1}^R (a_q \sum_{n=1}^N \phi_n^{r+q-2}) \quad r = 1 \dots R \quad (18)$$

The normal regression equations are the result of a mathematical treatment on the original polynomial, Equation 17. An explanation of the analysis may be found in statistics texts such as Hoel (Ref. 6).

Solution of these equations gives the set of "a" coefficients which minimize the residual sum of the squares:

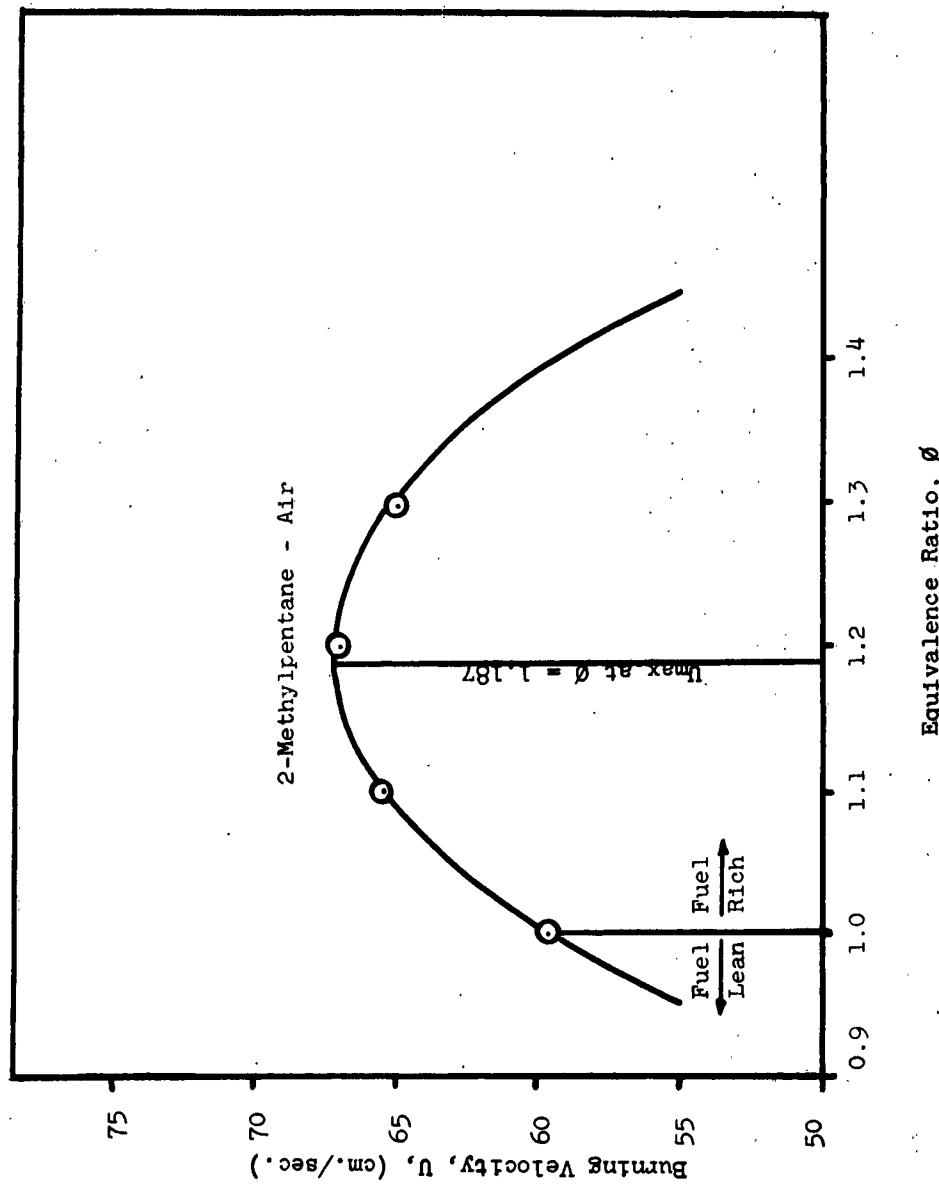


Fig. 3 Typical Curve Showing Burning Velocity,  $U$ , vs. Equivalence Ratio,  $\phi$

$$Q = \sum_{n=1}^N (u_n - \hat{u}_n)^2 \quad (19)$$

where  $\hat{u}_n$  represents a predicted value.

The standard deviation of  $u$  about  $\hat{u}$  is

$$S = \sqrt{Q/(N-R)} \quad \text{cm/sec} \quad (20)$$

If the calculated standard deviation is greater than the one specified, the cubic fit is declared unsatisfactory and a parabolic fit using Equation 18 with  $r=3$  is tried. If the standard deviation is still too high, the data set is ignored.

If only three points are available, a perfect parabolic fit,  $r=3$ , is obtained in the manner of Equation 17. Less than three points are not considered since they cannot define a curve with a maximum.

### (b) Equivalence ratios

(i) Cubic maximum Once the cubic fitting procedure has been satisfactorily completed, it is necessary to determine the maximum point  $(u_{\max}, \phi_{\max})$  of the curve. Two additional factors must be considered. The maximum velocity must occur within the data range considered, and a minimum velocity must not occur within the data range. If either of these conditions is violated, a parabolic fit is attempted.

Double differentiation of Equation 17 with  $r=4$  gives

$$\dot{\hat{u}} = a_2 + 2a_3\phi + 3a_4\phi^2 \quad (21)$$

$$\text{and } \ddot{\hat{u}} = 2a_3 + 6a_4\phi \quad (22)$$

At the maximum

$$\dot{\hat{u}}_{\max} = 0 \quad (23)$$

$$\text{and } \ddot{\hat{u}}_{\max} < 0 \quad (24)$$

Solving Equations 21 - 24 yields

$$\phi_{\max} = (a_3/3a_4)(1 \pm \sqrt{1-3a_2a_4/a_3^2}) \quad (25)$$

$$\text{and } 0 > \mp 2a_3 \sqrt{1-3a_2a_4/a_3^2} \quad (26)$$

The inequality shows that the upper sign is to be used in Equation 26 when  $a_3$  is positive, and vice versa.

For a real maximum to exist, three conditions must be fulfilled:

$$a_4 \neq 0 \quad (27)$$

$$a_3 \neq 0 \quad (28)$$

$$1 - 3a_2a_4/a_3^2 > 0 \quad (\text{real roots}) \quad (29)$$

(ii) Cubic minimum The equivalence ratio at the minimum point  $(\bar{\theta}_{\min}, \bar{u}_{\min})$  of the cubic equation must also be determined:

$$\bar{\theta}_{\min} = -(a_3/3a_4)(1 \pm \sqrt{1 - 3a_2a_4/a_3^2}) \quad (30)$$

The upper sign is understood to hold when  $a_3$  is positive, and vice versa. This equivalence ratio must not lie within the data range.

(iii) Parabolic maximum When a satisfactory parabolic fit is obtained,  $\bar{\theta}_{\max}$  is given by

$$\bar{\theta}_{\max} = -a_2/2a_3 \quad (31)$$

in which  $a_3$  must be negative.

### Function 3 (Executive routine)

- Given: (a) Combustion mixture temperature and pressure  
           (b) Fuel stoichiometric oxygen demand  
           (c) Mole fraction of  $O_2$  in oxidant  
           (d) Equivalence ratio at maximum flame speed

- Calculate: (a) Fuel concentration at maximum flame speed  
           (b) Fuel concentration at stoichiometric conditions

(a) Fuel concentration at  $u_{\max}$ ,  $(c_f)_{\max}$  For any value of the equivalence ratio  $\bar{\theta}$ , the fuel concentration is given by

$$c_f = \frac{(6.0238 \times 10^{23}) p_m}{62,366(t_m + 273.15)(1 + r_{st}/2\bar{\theta}z_{ox})} \quad (32)$$

molecules cc

Therefore  $(c_f)_{\max} = c_f$  evaluated at  $\phi = \phi_{\max}$  (33)

Similarly, (b) Fuel concentration at  $\phi = 1$ ,  $(c_f)_{stoc}$

$$(c_f)_{stoc} = c_f \text{ evaluated at } \phi = 1 \quad (34)$$

#### Function 4 (Executive Routine)

Given: (a) Results listed above  
(b) Composition, source, conditions and related input information

Action: Stores in memory only acceptable data groups

#### Function 5 (Subroutine Tape)

Given: (a) Acceptable groups stored in memory and on master tape 6  
(b) Changes to be made in the data already on the master tape

Action: (a) Edit the existing master tape data  
(b) Add new data groups to the master tape

In all cases, the input data, intermediate values, and output values are printed out at each step.

Function Options Four options are provided to permit portions of the program to be by-passed. The options would be exercised if portions of the experimental data had been processed previously or if outside data were to be used.

1. Complete calculation {Functions 1 through 4}
2. Partial calculation {Functions 2 through 4}
3. No calculation {Function 4}
4. Tape writing {Function 5 - follows successful execution of the other options}

#### FLAME SPEED REGRESSION CALCULATIONS (Routine FSR)

Functions Performed Routine FSR prepares the input data tape for the Esso Regression Analysis subroutine. Its operation may be considered in three stages:

### Function 1

Given: (a) All data groups currently stored on master tape 6.

(b) A list of data group accept/reject tests

Action: Selects and stores up to 300 data groups passing the accept/reject tests

Seven different tests are available for accepting or rejecting data groups now recorded on the master tape for the regression analysis. These tests may be employed in any combination desired, including omission of any or all. A limit of 300 acceptable data groups has been imposed for each regression run. If more than 300 could pass the tests, only the first 300 doing so are accepted for regression.

(a) Data group serial number test Those data groups whose serial numbers (machine assigned in order of tape position) are given in an input specification list are unacceptable.

(b) Fuel class test Only those data groups whose fuel class numbers are specified in an input list are acceptable.

(c) Fuel group test Only those data groups whose fuel class-group numbers are specified in an input list are acceptable.

(d) Fuel member test Only those data groups whose fuel class-group-member numbers are not specified in an input list are acceptable.

(e) Data source test Only those data groups whose source number corresponds to an input source number are acceptable.

(f) Experimental conditions test Only those data groups whose experimental conditions number corresponds to an input conditions number are acceptable.

(g) Contributor count tests Data groups may be acceptable or unacceptable depending on the presence or absence of given contributors in the fuel molecule. In addition, the counts of any specified contributors may be assumed zero whether they are zero or not on the master tape.

## Function 2

- Given:
- (a) All data groups selected as above
  - (b) Dependent variable numerator and denominator code numbers
  - (c) A list of prespecified coefficients with their corresponding contributor numbers

Calculate: Adjusted and scaled dependent variables for regression

(a) Dependent variable calculation The basic regression problem is to determine the  $b_u$  and  $b_o$  coefficients in the equation

$$y = b_o + \sum_u b_u n_u \quad (35)$$

such that the sum of the squares of the difference between the actual and predicted values is minimized. Routine FSR provides the option to define the dependent variable  $y$  provided the independent variables are still contributor counts. Thus, if regression of the maximum flame speed on contributor concentrations at maximum flame speed is desired,  $y$  would be defined

$$y = u_{\max} / (c_f)_{\max} \quad (36)$$

The dependent variable  $y$  may be any quantity expressible as a simple ratio of any two of the following quantities:

<u>Quantity</u>	<u>Identification Number</u>
1.0	1
$u_{\text{stoc}}$	2
$u_{\max}$	3
$(c_f)_{\text{stoc}}$	4
$(c_f)_{\max}$	5
$\emptyset_{\max}$	6

(b) Dependent variable adjustment If it is desired to prespecify (and therefore not calculate) some of the  $b$  coefficients in a given problem, it is necessary to adjust

the dependent variable by subtracting the contributions associated with the prespecified coefficients. Equation 37 indicates the procedure

$$y'_1 = y_1 - \sum_s b_s n_{1s} \quad (37)$$

(c) Dependent variable scaling To avoid exceeding the numerical limit of the computer ( $10^{38}$ ) during the regression calculations, all of the final dependent variables are scaled (i.e., multiplied by a constant factor)

$$Y_1 = y'_1 \cdot 10^E \quad (38)$$

so that the largest  $Y_1$  in a given problem does not exceed 1000.

### Function 3

Given: {a) All data obtained above  
{b) Input lists of overriding regression control data (optional)

Action: For each valid regression problem store on tape 7:

- {a) Output page heading
- {b) Regression control data
- {c) Independent variable values (contributor counts)
- {d) Adjusted and scaled dependent variable values

The regression analysis routine, a modification of SHARE E-R-MPR2, requires input data for the control of calculation and printing. One of the functions of routine FSR is to supply the needed data in the proper form. Although this is done automatically using internally stored values, input control data may be given if it is desired to override any of these values.

In all cases the important input data and intermediate and output values are printed for each function listed above.

## V. THE COMPUTER PROGRAM

### FLAME SPEED DATA REDUCTION (Routine FSC)

Routine FSC consists of an executive, or master control program and the eight subroutines listed below.

1. EXPD1
2. EXPD3
3. MAXM
4. TAPE
5. CROUT
6. INPUT
7. VDECOM
8. DECDP

Section IV contained a brief outline of the functions of the executive routine and the first four subroutines listed above. Here, these shall be discussed in more detail.

Executive Routine The executive routine controls the selection of five of the eight subroutines. The first data card in each group contains information regarding the option to be performed, the use of EXPD1 or EXPD3 and the use of MAXM. The executive routine reads this card and sequences the operations accordingly. Diagnostic code numbers are present in each of the subroutines and if any of these are exercised the executive routine will cause the printout of a diagnostic. If subroutine MAXM indicates that the data processed were satisfactory, the executive routine will store the pertinent values in memory prior to their addition to the master tape. Two small calculations,  $(cf)_{st}$  and  $(cf)_{max}$  are also made. It has been attempted to indicate each step in the actual program with "comment cards", and for convenience a nomenclature list precedes each routine. These can be found in Appendix A.

Subroutines EXPD1 and EXPD3 Both subroutines perform the same basic calculation of total cone area, flame speed, and equivalence ratio. However, the respective data outputs differ slightly. It was considered less confusing if each alternative had its own subroutine. Which subroutine to use is determined mainly by the intended use of the data after processing.

If the data to be processed are to be considered for addition to the master tape, subroutine EXPD1 should be used. In this subroutine, one experimental run number pertains to the entire data group and the input and output are set up accordingly.

If a set of control data are run sequentially, subroutine EXPD3 should be used. Each calculation is listed sequentially in the output to avoid confusion of the output with that from EXPD1. Sample printouts from both subroutines may be found in Appendix A.

Subroutines MAXM and CROUT Subroutine MAXM analyzes the data to see if either a valid cubic maximum or a parabolic maximum occurs within the data range. Subroutine CROUT solves the equations generated for the regression coefficients. As the logic used in subroutine MAXM is more involved than in the others, a brief stepwise description is presented.

1. If the number of experiments (or points) per data group is 1 or 2, signal that the data are "bad" and return to the executive routine. If there are 3 points, go to step 6; otherwise go to step 2.
2. Calculate the cubic coefficients either from the cubic polynomial (4 points) or from the "normal regression equations" (more than 4 points), as indicated in Section IV. If the calculation is successful, go to step 3; if not, to step 6.
3. Check cubic maxima criteria (coefficients zero or imaginary square root). If all are satisfied go to step 4; if not, to step 6.
4. Calculate  $\emptyset_{\max}$  and  $\emptyset_{\min}$ . Check for  $\emptyset_{\max}$  inside data range and  $\emptyset_{\min}$  outside data range of  $\emptyset$ . If so, go to step 5; if not, to step 6.
5. Calculate  $u_{stoc}$ ,  $u_{\max}$ ,  $\hat{u}_n$ , absolute and per cent differences between  $u_n$  and  $\hat{u}_n$ , and standard deviation S. If S is less than or equal to a specified value, signal the data "good" and return to the executive routine; if greater, signal the data "bad" and return to the executive routine.
6. Calculate the parabolic coefficients from the quadratic polynomial (3 point) or from the "normal regression equations" (more than 3 points). If the calculation succeeds, go to step 7; if not, to step 9.
7. Check for negative coefficient  $a_3$  (curve concave downwards). If so, calculate  $\emptyset_{\max}$  and go to step 8; if not, to step 9.

8. Check for  $\theta_{max}$  inside  $\emptyset$  data range. If so, go to step 5; if not, to step 9.

9. Signal the data "bad" and return to the executive routine.

Subroutine TAPE This subroutine controls all operations that change the contents of the master tape. The first portion of the routine scans the tape and makes the alterations to the data groups that were specified on an input data card. The second section permits the alteration or addition of contributor code numbers and names. The third section adds to the master tape the new data groups that were either approved by MAXM or entered via option 3. The final section is used only for the initial makeup of the master tape. Once the tape contains some data the other portions of the program may be used without a sequencing diagnostic.

Subroutines INPUT, VDECOM, and DECDP These subroutines facilitate preparation of the input data cards by permitting a variable width format. The complete card format is described in Section VI.

#### FLAME SPEED REGRESSION (Routine FSR)

Routine FSR prepares the input data for the E-R-MPR2 Esso Multiple Regression subroutine. It does not alter the input data (with the exception of scaling the dependent variable), but serves only for selecting the appropriate data for the regression analysis. In addition, control data are supplied for the Esso program.

Accept/Reject Tests Seven tests are provided for accepting or rejecting data groups. The first six tests are simple yes/no choices and were explained in Section IV. These tests are listed below.

1. Data group serial number test
2. Fuel class test
3. Fuel group test
4. Fuel member test
5. Data source test
6. Experimental conditions test

Test 7, the contributor count test, is more complicated and will be explained here in detail.

Data groups will be found acceptable or unacceptable depending upon the presence or absence of particular contributors in the fuel molecule. In addition, the counts of any contributor may be set equal to zero. The code numbers and test operation are listed below.

zero test - The count of the specified contributor(s) is set to zero

one test - The count of this contributor may be either zero or positive.

two test - The count of this contributor must be zero or the group will be rejected.

three test - The count of this contributor must be positive or the group will be rejected.

four to nine tests - Six tests are available to select data groups on the basis of a particular contributor content. The acceptance of a data group may be conditional upon it containing (+) and/or excluding (-) a certain number of a list of contributors. An example should clarify this.

#### Example

The data card types are given an alphabetic identification. The contributor count tests are specified on a "P" type card and the conditional tests on a "Q" type card.

(a) Sample P-type Card      1, 0, 15, 1,  
16, 0, 27, 4, 29, 5, 32, 3, 33, 5, 34,  
4, 37, 2, 40, 6, 61, 0.

#### Interpretation

Apply zero test (0) to contributors number 1-14, 16-26, 61 and up

Apply one test (1) to contributor number 15

Apply two test (2) to contributors number 37-39

Apply three test (3) to contributor number 32

The above tests are specific; the following are conditional:

Apply four test (4) to contributors  
number 27, 28, 34-36  
Apply five test (5) to contributors  
number 29-31, 33  
Apply six test (6) to contributors  
number 40, 41

(b) Corresponding Q-type Card

+3, -2, +1

Interpretation

Four test; the data group must contain (+) at least 3 contributors from the list 27, 28, 34-36.

Five test; the data group must not contain (-) at least 2 contributors from the list 29-31, 33.

Six test; the data group must contain either contributor 40 or 41.

NOTE: Conditional tests 7 to 9 were not used in the example.

Dependent Variable Limitations Up to 10 different dependent variables may be regressed in a single computer run (problem numbers 1 to 10). All problems in the same run share a common list of regression control data and operate on the same set of selected data groups.

Regression Control Data The regression analysis subroutine, a modification of SHARE E-R-MPR2, requires several pieces of information for the control of calculation and printing. One function of routine FSR is to supply the needed data in the proper form. This is done automatically using internally stored values. Only when it is desired to override one or more of the internal values is it necessary to supply input control data. Internally stored values are given in the following list.

<u>Item</u>	<u>Description</u>	<u>Built-in Value</u>
Dec. 1	Tolerance	0.001*
2	F value for entering variable	0.00002*
3	F value for removing variable	0.00001*
Int. 1	Problem number	calculated
2	Number of variables	calculated
3	Number of points (data groups)	calculated
4	Weighting factors given	1 (no)
5	Intermediate steps printed	0 (yes)*
6	Raw sums of squares and cross products printed	1 (no)*
7	Averages to be printed	1 (no)*
8	Residual sums of products to be printed	1 (no)*
9	Partial correlation coefficients to be printed	1 (no)*
10	Predicted values ( $Y_i$ 's) to be printed	0 (yes)*
11	Constant term ( $b_0$ ) to be assumed non-zero	1 (no)*

Values marked with an asterisk may be overridden by input values.

## VI. USE OF THE COMPUTER PROGRAMS

Both routines have been written in the standard FORTRAN II language compatible with most large-scale computing equipment. A maximum of four magnetic tape units are required in addition to any tape units used for input-output operations. The routines, as presented in Appendices A and B, are programmed to be compatible with the IBM 7090 Monitor system, with Tape 2 designated as the input and Tape 3 as the output.

Two additional routines have been included to avoid the storage of the master data tape over a period of time. Routine FSRDM will prepare a master data deck, or modify an existing data deck from information contained on the master data tape. Routine FSRTL will prepare a tape from the master data deck. These routines are presented in Appendix C.

### INPUT DATA DECK PREPARATION

The programs accept the standard IBM type, 80-column punched cards. However, only columns 1 to 72 may contain information to be processed by the computer. It is recommended that columns 73-80 be used for some type of identification both for the users standpoint as well as for the computing center.

All decimal input data and most integer input data are processed via subroutines VDECOM and DECDCP before being used in the computation portion of the main routine. The use of these subroutines simplifies data card preparation to the extent that field widths may be neglected. It is only necessary to provide a blank space or a comma between entries on the data cards. One restriction is imposed though. No entry may end in column 72 on the data card.

### FLAME SPEED DATA REDUCTION

The input data deck may consist of several sets of cards depending on the nature of the data and the option applicable. If only the calculated flame speed is of interest, an unlimited number of data sets may be entered. If, however, options 1, 2, or 3 are used for the purpose of adding data groups to the master tape, an option 4 must follow every 20 sets or less. This limitation is imposed because of the internal storage requirements of the program. Options 1, 2, or 3 may be run in any order.

To simplify the makeup of the data decks, each card fulfilling a specific purpose has been assigned an alphabetic code letter. Below are listed the data deck requirements for each of the options available. The actual makeup of the cards follows.

Option 1 Calculation of Flame Speeds from Raw Data

The first four card types set up the calculation sequence and define certain general conditions. The remaining cards contain the experimental measurements for each flame photograph. Thus, for a total of  $N_2$  photographs, the card order would be:

<u>Card Order</u>	<u>Card Type</u>
1	A
2	X
3	B
4	C
5 to $N_2 + 4$	D

Certain entries on the A card determine whether or not a full calculation or just the flame speeds are required. If the latter is the case, any number of these sets may be submitted, otherwise the maximum number before a tape writing sequence is 20.  $N_2$  is limited to 10.

Option 2 Calculations for Given Equivalence Ratios and Flame Speeds

The first four card types are similar to those mentioned above. The last card contains the predetermined flame speeds and equivalence ratios.

<u>Card Order</u>	<u>Card Type</u>
1	A
2	X
3	B
4	C
5	E

Option 3 All Final Values Given

Only the information on the first three card types is required.

<u>Card Order</u>	<u>Card Type</u>
1	A
2	X
3	B

#### Option 4 Tape Writing and Editing

The first card type remains the same. The second card type contains information about the remaining two card types.

<u>Card Order</u>	<u>Card Type</u>
1	A
2	F
3	G
4	H

Card Content by Card Type All numerical input data for routine FSC are processed by subroutines VDECOM and DECDCP. In the listings below, all integer quantities are designated Int. and all floating point quantities (e.g. .002 or 2.E-3 or 2.-3) are designated Dec. The only restrictions on preparation of these cards are that column 72 must be blank and each entry must be separated by at least one blank or comma. Readin of alphanumeric input is accomplished with an "A" format and the card column designations below must be maintained.

#### A Card

Entry 1	Int.	1000, card identification
2	Int.	Run number (1 to 9999)
3	Int.	4, number of integer entries following
4	Int.	Option number (1 to 4)
5	Int.	EXPD, subroutine number (1 or 3)
6	Int.	No., number of inhibitors present
7	Int.	MAXM, subroutine switch (0-use, 1-bypass)
8	Int.	1, number of decimal entries following
9	Dec.	0., dummy entry

#### X Card

	Columns	
Entry 1		Int. 0000, card identification
2		Int. 0, dummy entry
3		Int. 0, dummy entry
4	13-24	Alphabetic, fuel name
5	25-36	Alphabetic, date
6	37-48	Alphabetic, inhibitor name
7	49-60	Alphabetic, inhibitor name

A maximum of ten inhibitor names may be entered. These names must follow sequentially on the data cards and must occupy twelve columns per name. Columns 1 to 12 on each card, however, must contain the three integer entries listed above. Thus, if  $N_0$  were 4, the fuel name, data and three inhibitor names would go on the first X card while the fourth name would appear in Columns 13 to 25 of the second X card.

#### B Card

Entry 1	Int.	2000, card identification
2	Int.	Run number
3	Int.	7, number of integer entries following
4	Int.	Option number (1 to 3)
5	Int.	Fuel class number (0 to 99)
6	Int.	Fuel group number (0 to 99)
7	Int.	Fuel member number (0 to 99)
8	Int.	Data source number (1 to 9999)
9	Int.	Experimental condition number (1 to 9999)
10	Int.	$N_1$ , number of contributors listed on following B cards (1 to 100)
11	Int.	5, number of decimal entries following
12	Dec.	Flame speed at stoichiometric conditions (cm/sec)*
13	Dec.	Maximum flame speed (cm/sec)*
14	Dec.	Fuel concentration at stoichiometric conditions (molecules/cc)*
15	Dec.	Fuel concentration at maximum flame speed (molecules/cc)*
16	Dec.	Equivalence ratio at maximum flame speed*

\*Enter 0.0 when these values are not known (i.e., for options 1 and 2)

#### B Card Continuation

Entry 1	Int.	2001, card identification
2	Int.	Run number
3	Int.	$N_2$ , number of integer entries following ( $N_2 \leq 10$ )
4 to $N_2+3$	Int.	Contributor code numbers
$N_2+4$	Int.	$N_2$ , number of decimal entries following
$N_2+5$ to $2N_2+5$	Dec.	Contributor count

If more than ten contributors are present, additional continuation cards may be used. For each subsequent continuation card increase the card identification number by one (1).

C Card

Entry 1	Int.	3000, card identification
2	Int.	Run number
3	Int.	2, number of integer entries following
4	Int.	Option number (1 or 2)
5	Int.	$N_3$ , number of experiments in data group (EXPDL) or number of experimental runs (EXPD3) (i.e., number of D cards)
6	Int.	7, number of decimal entries following
7	Dec.	Mixture temperature ( $^{\circ}$ C)
8	Dec.	Mixture absolute pressure (mm Hg)
9	Dec.	Stoichiometric oxygen ratio (atoms oxygen/molecule fuel)
10	Dec.	Mole fraction $O_2$ in oxidant
11	Dec.	Volume per mole of fuel at given fuel flow rates (cc/gram-mole)
12	Dec.	Maximum allowable standard deviation in u vs. $\phi$ curve for addition to tape (assumed 1.0 cm/sec if 0.0 entered)
13	Dec.	Actual distance between teeth tips seen on schlieren photograph (cm) (assumed to be 0.2 cm if 0.0 entered)

D Card

Entry 1	Int.	4000, card identification
2	Int.	Run number
3	Int.	2, number of integer entries following
4	Int.	1, option number
5	Int.	$N_4$ , number of diameter measurements listed on continuation card (1 to 100)
6	Int.	6, number of decimal entries following
7	Dec.	Fuel flow at mole volume of entry 11 on C card
8	Dec.	Oxidant flow at STP (cc/sec)
9	Dec.	Mole fraction of inhibitor in final mixture
10	Dec.	Measured peak height (arbitrary units)
11	Dec.	Reference length (cm)
12	Dec.	Reference length (arbitrary units)

D Card Continuation

Entry	1	Int.	4001, card identification
	2	Int.*	Run number
	3	Int.	$N_5$ , number of integer entries following
	4 to $N_5 + 3$	Int.**	Station height of diameter measure- ment (1 = cone base)
	$N_5 + 5$ to $2N_5 + 5$		Cone diameter (arbitrary units)

\*For data processing by subroutine EXPD1, the run number on each D card must be the same as that on the A, B and C cards. For processing by routine EXPD3, the run number is to be incremented by one for each subsequent D card.

\*\*The station heights correspond to the "teeth locations referred to in the C card description. The distance between twenty reference teeth was accurately known. As all flame speed measurements were made on a microfilm reader, it was found to be more accurate and more convenient to measure the flame diameters and teeth spacing in any suitable units (say mm) and have the computer rescale the measurements to the desired units.

E Card

Entry	1	Int.	5000, card identification
	2	Int.	Run number
	3	Int.	1, number of integer entries following
	4	Int.	2, option number
	5	Int.	$N_3$ , number of flame speed - equivalence ratio entries (1 - 10)

E Card Continuation

Entry	1	Int.	5001, card identification
	2	Int.	Run number
	3	Int.	1, number of integer entries following
	4	Int.	0, dummy entry
	5	Int.*	$N_3$ , number of flame speed equivalence ratio entries
	6 to $6 + N_3$	Dec.	

\* $N_3$  is entry 5 on the C card and must not have a value exceeding 10.

F Card

Entry	1	Int.	6000, card identification
	2	Int.	Run number
	3	Int.	5, number of integer entries following
	4	Int.	4, option number
	5	Int.	$N_6$ , number of G-card groupings to follow (0 to 20)(contributor count changes)
	6	Int.	$N_7$ , number of entry pairs on H-card (0 to 50)(contributor name changes)
	7	Int.	7, for initial tape makeup, otherwise zero
	8	Int.	0, for other than last data card set; 1, for last set
	9	Int.	1, number of decimal entries to follow
	10	Dec.	0., dummy entry

G Card

Entry	1	Int.	7000, card identification
	2	Int.	Run number
	3	Int.	2, number of integer entries following
	4	Int.	Data group serial number
	5	Int.	$N_8$ , number of entry pairs in contributor count change list (0 to 90)
	6	Int.	1, number of decimal entries following
	7	Dec.	0., dummy entry

G Card Continuation

Entry	1	Int.	7001, card identification
	2	Int.	Run number
	3	Int.*	$N_9$ , number of integer entries following (0 to 10)
	4 to $N_9+3$	Int.	Contributor number
	$N_9+4$	Int.	$N_9$ , number of decimal entries following
	$N_9+5$ to $4+2N_9$	Dec.	Contributor count

\*If  $N_9 > 10$  additional continuation cards will be required. The card identification number must be incremented by one on each continuation card.

H Card

Columns 1 to 4	0000
6	0
8	0
13 - 16	contributor number
25 - 28	contributor number
...	
61 - 64	contributor number
* { 19 - 24	alphabetic contributor name
31 - 36	alphabetic contributor name
...	
67 - 72	alphabetic contributor name

\*There are to be five entry pairs per H card. If  $N_7$  from the F card is greater than 5, continue the listing on additional cards at five pairs per card.

Fortran Routine The Fortran II program is listed in Appendix A with sample printouts. Duplicate decks of this program are available.

FLAME SPEED REGRESSION

The number and type of cards comprising the data deck will depend upon the number of tests and changes wanted. To facilitate the deck makeup, each specific data card has been given an alphabetic code letter from I through U. Card types I, J, K, and T in the deck are mandatory with the K-type card containing control integers governing the number and type of all but one of the remaining cards.

<u>Card Order</u>	<u>Card Type</u>
1	I
2	J
3	K
Next, unless $N_2 = 0$	L
Next, unless $N_3 = 0$	M
Next, unless $N_4 = 0$	N
Next, unless $N_5 = 0$	O
Next, unless $N_6 = 0$	P

<u>Card Order</u>	<u>Card Type</u>
Next, unless $N_7 = 0$	Q
Next, unless $N_8 = 0$	R
Next, unless $N_9 = 0$	S
Next	T } *
Next, unless $N_{10} = 0$	U }

\* $N_1$  pairs of these cards may be used ( $N_1 \leq 10$ ). The T card contains  $N_{10}$  and hence governs the use of the U type card.

Card Content by Card Type With exception of the I, J, R and U type cards, all input data to routine FSR are integers. A fixed format is used to accomplish this with four spaces allotted to each entry (18I4). The type U cards are decomposed in subroutines VDECOM and DECDCP with the same limitations as described for routine FSC. When card column designations are given, they must be adhered to.

#### I Card - Subtitle Information for Routine FSR Printout

Column	1	Alpha	Blank
	2-72	Alpha	Subtitle

#### J Card - Title for Regression Program Printout

Column	1	Alpha	One (1)
Column	2-72	Alpha	Title

#### K Card - Routine FSR Control Card

Entry	1	Int.	Regression run number (1 to 9999)
	2	Int.	$N_1$ , number of dependent variable choices in this run
	3	Int.	$N_2$ , number of entries in input list (L card) of unacceptable data group serial numbers (0 to 300)
	4	Int.	$N_3$ , number of entries in input list (M card) of acceptable fuel class numbers () to 13)
	5	Int.	$N_4$ , number of entries in input list (N card) of acceptable fuel class group numbers (0 to 40)
	6	Int.	$N_5$ , number of entries in input list (O card) of unacceptable fuel class-group-member numbers (0 to 80)
	7	Int.	Acceptable data source number (0 to 999, 0 means all sources acceptable)

Entry	8	Int.	Acceptable experimental conditions number (0 to 999, 0 means all conditions acceptable)
	9	Int.	$N_6$ , number of entry pairs in input list (P card) of contributor count tests (0 to 200)
	10	Int.	$N_7$ , number of entries in input list (Q card) of conditional count test criteria (0 to 6)
	11	Int.	$N_8$ , one if overriding decimal regression control data (R card) to be read; otherwise zero
	12	Int.	$N_9$ , number of entry pairs in input list (S card) of overriding integer regression control data (0 to 7)
	13	Int.	Highest contributor number in use (1 to 200, higher ones ignored)
	14	Int.	1, for the last run, otherwise zero

L Card

Entry 1 to $N_2$	Int.	Unacceptable data group serial numbers ( $N_2 \geq 300$ )
------------------	------	---

M Card

Entry 1 to $N_3$	Int.	Acceptable fuel class numbers ( $N_3 \leq 20$ )
------------------	------	---

N Card

Entry 1 to $2N_4$	Int.	Acceptable fuel class-group numbers ( $N_4 \leq 40$ ) paired.
-------------------	------	---

O Card

Entry 1 to $3N_5$	Int.	Unacceptable fuel class-group-members ( $N_5 \geq 80$ ) in trios.
-------------------	------	---

P Card (see "Contributor Count Tests")

Entry 1,3 $2N_6-1$	Int.	Contributor number $N_6$ pairs
2,4 $2N_6$	Int.	Contributor count test ( $N_6 \leq 200$ )

Q Card

Entry 1 to $N_7$	Int.	Conditional count test criteria. First entry goes with test 4, second with 5, etc. ( $N_7 \leq 6$ )
------------------	------	--

R Card (see "Regression Control Data")

Columns 1 to 10 Dec.      Tolerance  
11 to 20 Dec.      F value for entering variable  
21 to 30 Dec.      F value for removing variable

S Card (see "Regression Control Data")

Entry 1,3  $2N_9 - 1$  Int.      Integer regression control item  
number  
2,4  $2N_9$       Int.      Overriding integer regression       $N_9 \leq 7$   
control data

T Card

Entry 1      Int.      Dependent variable numerator  
identification number (1 to 6)  
2      Int.      Dependent variable denominator  
identification number (1 to 6)  
3      Int.       $N_{10}$ , number of entry pairs in input  
list (U card) of prespecified re-  
gression coefficients for this  
problem (0 to 50)

U Card

Entry 1      Int.      1, card number  
2      Int.      Run number  
3      Int.\*       $N_{11}$ , number of integer and decimal  
pairs to follow  
4 to  $3+N_{11}$       Int.      Contributor number  
 $N_{11} + 4$       Int.       $N_{11}$   
 $N_{11} + 5$  to  $4+2N_{11}$       Dec.      Prespecified coefficient

\*If  $N_{10} > 10$  additional U type cards will be required until  
all of the contributor numbers and coefficients are entered.  
The card number must be incremented by one for each additional  
card.

Fortran Routine      The Fortran II program for routine FSR  
is listed in Appendix B. Duplicate decks of this program are  
available.

MASTER DATA DECK LOADING AND MODIFICATION

Routine FSRTL      The only data cards required by the  
routine are those of the master data deck itself. The card  
image of this deck will be read onto logical tape 6 which  
will then be given an end of file and rewound.

Routine FSRDM If it is desired to update the master data deck, routine FSRDM will cause any or all of the data groups on the master tape to be punched. The master tape must be logical tape 6. All control data for the routine are integers and a fixed format is used which provides a six-column field width (12I6).

First control card for Routine FSRDM

Entry	1	Int.	Number of data groups in the master data card deck
	2	Int.	$N_1$ , number of data groups which have been altered since last deck makeup
	3	Int.	Punch contributor name list? (1-yes, 2-no)
	4	Int.	Punch dependent variable name list? (1-yes, 2-no)

If none of the data groups have been modified,  $N_1 = 0$  and the routine will punch only those data groups added since the last makeup. If  $N_1 \neq 0$  an additional control card is required.

Second control card for Routine FSRDM

Entry 1 to  $N_1$  Int. Serial number of data groups that have been modified since last deck makeup.

The Fortran II programs for routines FSRTL and FSRDM are listed in Appendix C. Duplicate decks of these programs are available.

## VII. NOMENCLATURE

a	Power series fitted coefficient
A	Area of flame schlieren cone, cm <sup>2</sup>
b	Regression coefficient
c	Number concentration, cm <sup>-3</sup>
D	Diameter of flame schlieren cone, cm
E	Dependent variable scaling exponent
h	Height above burner port, cm
n	Contributor count, no./molecule
N	A number
p	Absolute pressure, mm Hg
q	Volumetric flow rate, cm <sup>3</sup> /sec.
Q	Residual sum of squared differences
r	Atoms of oxygen per molecule of fuel
R	Maximum value of r subscript
S	Standard deviation
t	Temperature, °C
u	Flame speed, cm/sec.
v	Molar volume, cm <sup>3</sup> /g-mole
w	Molar flow rate, g-moles/sec.
x	Independent variable
y	Dependent variable
Y	Adjusted and scaled dependent variable
z	Mole fraction
Δ	Increment prefix
π	3.14159 ...
Ø	Equivalence ratio

### Subscripts

f	Of fuel
i	Data group index, block regression
j	Contributor index (or number)
m	Of combustible mixture
min	At minimum of cubic fitting equation
max	At maximum flame speed
n	Height index
o	Of oxygen, or zero index
p	At peak of flame cone
q	Dummy r index
r	Term index, u-Ø curve
s	Specified (or prespecified)
stoc	Stoichiometric
u	Unspecified (to be calculated by regression)
x	In oxidant

Superscripts

- ^ Calculated from a fitted equation
- \* At STP (0°C, 760 mm Hg abs.)
- ' Adjusted
- . First derivative
- .. Second derivative

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APPENDIX A

Fortran Program and Sample Printouts  
for Routine FSC

## ROUTINE FSCX

## FLAME SPEED CALCULATION EXECUTIVE PROGRAM

```

FSCX 2010 FEB 20 ,1962 FLAME SPEED CALCULATIONS MOD 2      1
C   EXECUTIVE ROUTINE FOR FLAME SPEED CALCULATIONS MRC - DAYTON  2
C   .                                         .                         3
C   .                                         .                         4
C   NOMENCLATURE  .                         .                         5
C   .                                         .                         6
C   A1(I) AND A2(I) - FUEL NAME  .                         7
C   NALK(L) - NUMBER OF STRUCTURAL CONTRIBUTORS PER MOLECULE  8
C   CNX - FUEL CONCENTRATION AT MAXIMUM FLAME VELOCITY        9
C   (MOLECULES / CC.)  .                         10
C   CSTOC - FUEL CONCENTRATION AT STOICHIOMETRIC           11
C   CONDITIONS (MOLECULES / CC.)  .                         12
C   DU AND TE - FIRST AND SECOND HALVES OF DATE  .             13
C   I, K, AND N - COUNTING INTEGERS  .                         14
C   IIA(I) - FUEL CLASS NUMBER  .                         15
C   IIB(I) - FUEL GROUP NUMBER  .                         16
C   IIC(I) - FUEL MEMBER NUMBER  .                         17
C   IJL,IY - DATA_SOURCE_NUMBER  .                         18
C   IS(I) - EXPERIMENTAL CONDITIONS NUMBER  .             19
C   I4(I) - NUMBER OF STRUCTURAL CONTRIBUTORS CONSIDERED  20
C   IADD - NUMBER OF DATA GROUPS ACCEPTABLE FOR WRITING  21
C   ICANT - OPTION_CONTROL_INTEGER CHECK  .               22
C   ICTL - OPTION CONTROL INTEGER  .                         23
C   IEXPD - EXPD_ SUBROUTINE_SELECTION_INTEGER  .          24
C   INHIB1(I,J) AND  .                         .                         25
C   INHIB2(J,I) - INHIBITION NAMES  .                         26
C   IPN - NUMBER OF EXPERIMENTS  .                         27
C   JILK(I) - SPECIES CONTRIBUTOR_CODE NUMBER  .           28
C   KODE - SIGNAL INTEGER FOR ACCEPTABLE DATA  .           29
C   NNUK - RUN NUMBER OF DATA GROUP  .                         30
C   NRUNT - RUN NUMBER CHECK  .                         31
C   O(I) - EQUIVALENCE RATIOS  .                         32
C   NUMINH - NUMBER OF INHIBITORS USED  .             33
C   OISK - ACTIONS OF OXYGEN TO COMPLETELY OXIDIZE ONE  34
C   OMX - MOLECULE OF FUEL  .                         35
C   PM - EQUIVALENCE RATIO AT MAXIMUM FLAME VELOCITY  36
C   PS - ABSOLUTE PRESSURE OF GAS MIXTURE (MM. MERCURY)  37
C   STDS - MAXIMUM ALLOWABLE STANDARD DEVIATION OF U VS  38
C   U - CURVE FOR ADDITION TO TAPE  .             39
C   D AND D(N) - EQUIVALENCE_RATIO  .             40
C   U AND U(N) - FLAME SPEED (CM./SEC)  .             41
C   TEETH - ACTUAL DISTANCE BETWEEN TEETH TIPS SEEN ON  42
C   SCHLIEREN PHOTOGRAPH (CM.)  .                         43
C   TM - MIXTURE TEMPERATURE (DEG. C)  .             44
C   UNK - MAXIMUM FLAME SPEED (CM./SEC)  .             45
C   USTOC - FLAME SPEED AT STOICHIOMETRIC CONDITIONS  46
C   (CM./SEC)  .                         .                         47
C   VBFO - VOLUME PER MOLE OF FUEL (CC./GRAM-MOLE)  48
C   VBM - VOLUME PER MOLE OF MIXTURE (CC./GRAM-MOLE)  49
C   YOK - MOLE FRACTION OXYGEN IN OXIDANT  .             50
C   .                                         .                         51
C   .                                         .                         52
C   COMMON INT, DEC, IC, J1, J2, JS, NIN, NEX  .             53
C   DIMENSION INT(10), DEC(10)  .                         54
C   DIMENSION A1(20),A2(20),B1(100,20),DA(6,20),IIA(20),IIB(20),  55
C   1     IIC(20),IJ(20),IJ3(20),IJ4(20),J1(100,20),O(10),U(10)  56
C   2     ,INHIB1(10,20),INHIB2(10,20)  .             57
C   NIN = 1  .                         .                         58
C   20 IADD = 0  .                         .                         59
C   30 CALL INPUT  .                         .                         60
C   NEX = NEX  .                         .                         61
C   GO TO 1, 521, 701, 300, 901, 300, 300, 300, NEX  .             62
C   .                                         .                         63
C   .                                         .                         64
C   .                                         .                         65
C   .                                         .                         66
C   .                                         .                         67
C   .                                         .                         68
C   .                                         .                         69
C   .                                         .                         70
C   IF (NRUN) 32,210,32  .                         71
C   32,IF(NUMINH) 320,320,33  .                         72
C   320 NUMINH = '1'  .                         73
C   .                                         .                         74
C   .                                         .                         75
C   .                                         .                         76
C   33 IF (ICLT = 4) 40,150,30  .                         77
C   40,IF (ICLT) 40,30,50  .                         78
C   50 I = IADD + 1  .                         79
C   .                                         .                         80
C   .                                         .                         81
C   .                                         .                         82
C   52 READ INPUT TAPE 2, 1002  .                         83
C   9     , A1(I),A2(I),DU,TF ,INHIB1(J,I),INHIB2(J,I),J=1,  .             84
C   INUMINH)  .                         85
C   GO TO 30  .                         .                         86
C   .                                         .                         87
C   .                                         .                         88
C   .                                         .                         89
C   .                                         .                         90
C   521,NUMCON = IC = 2000  .                         91
C   IF (NUMCON) 523, 522, 523  .                         92
C   NRUNT = J11  .                         .                         93
C   .                                         .                         94
C   .                                         .                         95
C   .                                         .                         96
C   .                                         .                         97
C   .                                         .                         98
C   .                                         .                         99
C   K1 = INT(7)  .                         .                         100
C   00 5220 K = DEC(K-1)  .                         101
C   GO TO 30  .                         .                         102
C   523 IF (NRUNT = J11) 300, 5230, 300  .             103
C   5230 LIMIT = 109_NUMCON  .                         104
C   GO = LIMIT = 9  .                         .                         105
C   IF(LIMIT = K1) 523, 523, 524  .             106

```

## FLAME SPEED CALCULATION EXECUTIVE PROGRAM

```

524 LIMIT = K1          FSCX 107
525 M = 0              FSCX 108
526 DO 526_K = JGO, LIMIT FSCX 109
      M = M + 1          FSCX 110
      J1(K1) = INT(M)    FSCX 111
      526_B1(K1) = DEC(M) FSCX 112
      IF( LIMIT - K1 ) .GT. 52_30 FSCX 113
      53_I4(I) = K1       FSCX 114
      FSCX 115
C   PRINTOUT OF INPUT DATA FSCX 116
C   WRITE_OUTPUT TAPE 3, 1010 FSCX 117
      V , NRUN,DU,TE     FSCX 118
      WRITE_OUTPUT TAPE 3, 1011 FSCX 119
      WRITE_OUTPUT TAPE 3, 1012 FSCX 120
      9 , A1(I), A2(I), (INHIB1(J,I), INHIB2(J,I),J=1, NUMINH) FSCX 121
      WRITE_OUTPUT TAPE 3, 1013 FSCX 122
      9 , I1(I), I2(I), I3(I) FSCX 123
      WRITE_OUTPUT TAPE 3, 1014 FSCX 124
      9 , (DAK,I), K2,6) FSCX 125
      WRITE_OUTPUT TAPE 3, 1015 FSCX 126
      9 , IJ1(K1,I),B1(I,K1),K=1,K1) FSCX 127
      FSCX 128
C   RUN_NUMBER CONSISTENCY CHECK FSCX 129
      IF (NRUN - NRUNI) .NE. 200,55,200 FSCX 130
      FSCX 131
C   CONTROL INTEGER CHECK FSCX 132
      FSCX 133
C   55 IF (ICTL - ICANT) 200,60,200 FSCX 134
      FSCX 135
C   OPTION SELECTION FSCX 136
      60 IF (ICCTL - 2) 70,70,120 FSCX 137
      70 GO TO 30 FSCX 138
      FSCX 139
C   C CARD ASSIGNMENTS FSCX 140
      FSCX 141
C   701 NRUNT = J11 FSCX 142
      ICANT = INT(I) FSCX 143
      IPN = INT(2) FSCX 144
      TM = DEC(1) FSCX 145
      PM = DEC(2) FSCX 146
      DFSR = DEC(3) FSCX 147
      YOX = DEC(4) FSCX 148
      VBFQ = DEC(5) FSCX 149
      STD5 = DEC(6) FSCX 150
      TEETH = DEC(7) FSCX 151
      74 WRITE_OUTPUT TAPE 3,1017 FSCX 152
      WRITE_OUTPUT TAPE 3,1019 FSCX 153
      9 , TM,PM,DFSR,YOX,VBFQ FSCX 154
C   RUN NUMBER CONSISTENCY CHECK FSCX 155
C   IF (NRUN - NRUNI) .NE. 200,71,200 FSCX 156
      FSCX 157
C   CONTROL INTEGER CHECK FSCX 158
C   71 IF (ICCTL - ICANT) 200,75,200 FSCX 159
      75 VBM = 62366.0*(TM + 27.5)/PM FSCX 160
      CSTOC = 6.0238E23/(VBM*(L,0 + DFSR*(2.0+YOX))) FSCX 161
      FSCX 162
C   EXPERIMENTAL DATA PROCESSING FSCX 163
      FSCX 164
C   GO_TC_(80,90), ICTL FSCX 165
      80 GO_TC_(82,83,83), IEVD FSCX 166
      82 CALL EXPD(NRUN,ICTL,DFSR,YOX,VBFQ ,VBM, IPN, O, U, KODE, TEETH) FSCX 167
      1 NRUNT ) FSCX 168
      GO_TC_ 84 FSCX 169
      83 CALL EXPD(NRUN,ICTL,DFSR,YOX,VBFQ ,VBM, IPN, O, U, KODE, TEETH) FSCX 170
      1 NRUNT ) FSCX 171
      84 IF (KODE .EQ. 81) 81,100, 81 FSCX 172
      90 GO_TC_ 84 FSCX 173
      FSCX 174
C   E CARD ASSIGNMENTS FSCX 175
      FSCX 176
C   901 NUMCON = IC - 5000 FSCX 177
      IF( NUMCON ) 904, 902, 904 FSCX 178
      902_NRUNT = J11 FSCX 179
      ICANT = INT(I) FSCX 180
      DO 903 M = 1, IPN FSCX 181
      903_OIN = DEC(IN) FSCX 182
      GO_TO 30 FSCX 183
      904 DO 905 N = 1, IPN FSCX 184
      905_UIN = DEC(IN) FSCX 185
      FSCX 186
C   RUN NUMBER CONSISTENCY CHECK FSCX 187
      FSCX 188
C   IF (NRUN - NRUNI) .NE. 200,91,200 FSCX 189
      FSCX 190
C   CONTROL INTEGER CHECK FSCX 191
      FSCX 192
      91 IF (ICCTL - ICANT) 200,100,200 FSCX 193
      FSCX 194
C   DETERMINATION_OF_MAXIMUM_FLAME_SPEED FSCX 195
      FSCX 196
C   100_CALL MAXM_(IPN, O, U, DMX, UNK, USTOC, KODE, STD5, IEVD, MAXON, FSCX 197
      1 NRUN) FSCX 198
      FSCX 199
C   TEST FOR SUCCESSFUL DETERMINATION OF MAXIMUM FLAME SPEED FSCX 200
      FSCX 201
      IF (KODE .EQ. 31) 30,110,30 FSCX 202
      FSCX 203
      FSCX 204
C   TEST FOR REASON FOR UNSUCCESSFUL DETERMINATION OF MAX SPEED FSCX 205
      FSCX 206
      30 IF (KODE .EQ. 11) 30,200,30 FSCX 207
      110 CMX = 6.0238E23/(VBM*(L,0 + DFSR*(DMX+YOX*2.0))) FSCX 208
      FSCX 209
      FSCX 210
      FSCX 211
      FSCX 212

```

**ROUTINE FSCX**

(CONTINUED)

## **FLAME SPEED CALCULATION EXECUTIVE PROGRAM**

C STORAGE OF ACCEPTABLE DATA  
 DA12,I) = USTOC  
 DA13,I) = URM  
 DA14,I) = CSTOC  
 DA15,I) = CMK  
 DA16,I) = DMA  
 120 IADD = IADD + 1  
 C PRINTOUT OF ACCEPTABLE DATA  
 WRITE OUTPUT TAPE 3, 1020  
 WRITE OUTPUT TAPE 3, 1012  
 9 . A1(I), A2(I), (INHIB1(J,I), INHIB2(J,I), J-1, NUMINH)  
 WRITE OUTPUT TAPE 3, 1013  
 9 . I1(A1), I2(A2), I3(C1), I4(I), I5(I)  
 WRITE OUTPUT TAPE 3, 10131  
 9 . (DA1X,I,K=2,6)  
 GO TO 30  
 C TAPE EDITING AND WRITING  
 150 CALL TAPE (NRUN,ICTL,A1,A2,IAA,IBB,IIC,IC2,IC3,OA,IA,J1,B1,  
 1 (ADD, DU, TE, LAST)  
 C TEST FOR COMPLETION OF TAPE EDITING AND WRITING  
 C IF LASTI(15A)=20,L51  
 151 REMIND 8  
 210 WRITE OUTPUT TAPE 3, 1030  
 GO TO 20  
 C ERROR PRINT - RUN NUMBER OR CONTROL INTEGER INCONSISTENCY  
 200 WRITE OUTPUT TAPE 3, 1016  
 9 . NRUN,NRUNIT,ICTL,ICANT  
 GO TO 30  
 C DIAGNOSTIC - UNACCEPTABLE CARD ORDER  
 300 WRITE OUTPUT TAPE 3, 3000, IC, J11  
 NIN..2.  
 GO TO 30  
 C FORMAT STATEMENTS  
 1002 FORMAT ( 12X, 10A6 )  
 1010 FORMAT  
 9 (1H1, 97HMONGANTO RESEARCH CORPORATION FLAME SPEED CALCULATI  
 JON - ROUTINE 2018 MODIFICATION 1 RUN 14.6H DATE 2AB )  
 1011 FORMAT  
 9 ( 1H0, .25X,10HINPUT DATA )  
 1012 FORMAT  
 9 ( 1H0, 30X, 9HFUEL NAME , 35X, 1SHINHIBITORS USED //  
 1 . 1H0, 30X, 2A6, 32X,2A6 / (1H0, 74X, 2A6 )  
 1013 FORMAT  
 9 ( 1H0, .10X, .18HFUEL CLASS NUMBER 3X, 16, 1I1X,  
 1 . .18HFUEL GROUP NUMBER 3X, 16, 1I1X  
 2 . .18HFUEL MEMBER NUMBER 3X, 16, /  
 3 . 1H0, 10X, .10HDATA SOURCE NUMBER 3X, 16, 1I1X  
 4 . .30HEXPERIMENTAL CONDITIONS NUMBER 3X,16 )  
 10131 FORMAT  
 9 ( 1H0, .10X, .52HFAME VELOCITY AT STOICHIOMETRIC CONCENTRATION RATIO  
 10 . 3X, F9.4, 9X, 7HCM./SEC  
 2 1H0,10X, .22HMAXIMUM FLAME VELOCITY .33X, F9.4, 9X,7HCM./SEC /  
 3 1H0, 10X, .47HFUEL CONCENTRATION AT STOICHIOMETRIC CONDITIONS  
 4 . 10X, E13.6, 3X, .13HMOLECULES/CC  
 5 1H0, 10X, .52HFUEL CONCENTRATION AT CONDITIONS OF MAXIMUM VELOC  
 6Y . 5X, E13.6, 3X, .13HMOLECULES/CC /  
 7 1H0,10X, .40EQUivalence RATIO AT MAXIMUM FLAME SPEED 16X,F9.5 )  
 1014 FORMAT  
 9 ( 1H0, 16X,31HSPECIES CONTRIBUTOR CODE NUMBER  
 1 . 17X,43HNUMBER OF CONTRIBUTORS PER MOLECULE OF FUEL )  
 1015 FORMAT  
 9 ( 1H . 27X, 16, .49X, F8.3 )  
 1016 FORMAT  
 9 . 1H0, 16X,.30HDATA OUT\_OF\_ORDER - RUN NUMBER 14,  
 1 . 14X, .20HMISSPLACED RUN NUMBER 14,  
 2 / 1H0, 16X,.22HCONTROL CONTROL INTEGER 14,  
 3 . 22X,21HCONTROL INTEGER CHECK 14 )  
 1017 FORMAT  
 9 ( 1H, .25X, 17HEXPERIMENTAL DATA / )  
 1019 FORMAT  
 9 ( 1H0, 16X, .19HMIXTURE TEMPERATURE 3X, F6.1, 3X, 7HDEG. C.  
 1 . 14X, .16HMIXTURE PRESSURE 3X, F6.1, 3X, 1HMM, MERCURY /  
 2 1H0, 16X, .58HATOMS OF OXYGEN TO COMPLETELY OXIDIZE ONE MOLECULE  
 30F FUEL\_F,6.2 /  
 4 1H0, 16X, .23HMOLE FRACTION OXYGEN IN OXIDANT 3X, F7.4 /  
 5 1H0, 16X, .23HVOLUME PER MOLE OF FUEL 3X,1PE12.4,3X,17HCC., PER GRA  
 6M-MOLE )  
 1020 FORMAT  
 9 ( 1H, .25X,15HDATA ACCEPTABLE )  
 1030 FORMAT ( 1H1, 10X, 23HCOMPUTATIONS COMPLETED )  
 3000 FORMAT( 1H0, 25X, 41HDATA CARD ORDER INCORRECT - CARD NUMBER  
 1 . 14, .5X, 12HRun\_Number ..15 )  
 END

## SUBROUTINE EXPD1

## EXPERIMENTAL FLAME SPEED DATA REDUCTION

```

EXPDI EXPD1 SUBROUTINE MDO 0 MARCH 1, 1962 NRC-DAYTON          EXPDI  1
C      NOMENCLATURE                                         EXPDI  2
C      AR      - CUMULATIVE CONE AREA *2/PI                  EXPDI  3
C      AIN(J)   - TOTAL CONE AREA (SQUARE CM.)                EXPDI  4
C      DI(K)    - CONE DIAMETER AT ABOVE ELEVATION (CM.)     EXPDI  5
C      DAI(K)   - MEASURED DIAMETER AT ABOVE ELEVATION       EXPDI  6
C      DELS    - INCREMENT SLANT HEIGHT (CM.)                 EXPDI  7
C      ELA     - REFERENCE LENGTH MEASURED IN UNITS OF DAI(K) EXPDI  8
C      ELCM    - REFERENCE LENGTH MEASURED IN CM.             EXPDI  9
C      FMI(N)   - MOLE FRACTION OF INHIBITOR IN MIXTURE       EXPDI 10
C      H(K)    - ELEVATION ABOVE BURNER TOP (CM.)            EXPDI 11
C      HPKA    - MEASURED PEAK HEIGHT                         EXPDI 12
C      ICANT   - OPTION CONTROL INTEGER CHECK                EXPDI 13
C      IRK     - MEASURED ELEVATION ABOVE BURNER TOP          EXPDI 14
C      IPK     - TOTAL NUMBER OF CONE MEASUREMENTS           EXPDI 15
C      IPN     - NUMBER OF EXPERIMENTS                      EXPDI 16
C      IRK     - NUMBER OF DIAMETER MEASUREMENTS PER RUN    EXPDI 17
C      KODE    - SIGNAL INTEGER FOR ACCEPTABLE DATA          EXPDI 18
C      NRUN    - RUN NUMBER OF DATA GROUP                     EXPDI 19
C      NRUNT   - RUN NUMBER CHECK                           EXPDI 20
C      O(D AND OIN) - EQUIVALENCE RATIO                   EXPDI 21
C      OFSR    - ATOMS OF OXYGEN TO COMPLETELY OXIDIZE ONE   EXPDI 22
C      OFSR    - MOLECULE OF FUEL                          EXPDI 23
C      OFO(IN)  - FUEL FLOW (CC./SEC. AT VBFO MOLAR VOLUME) EXPDI 24
C      UMIN(N) - VOLUME FLOW OF MIXTURE (CC./SEC AT ACTUAL  EXPDI 25
C                  TEMPERATURE AND PRESSURE)                 EXPDI 26
C      QXO(IN)  - OXIDANT FLOW (CC./SEC AT 0 DEG. C, 760 MM. HG) EXPDI 27
C      SF      - SCALE FACTOR (CM./UNITS_OF_DAI(K))          EXPDI 28
C      TEETH   - ACTUAL DISTANCE BETWEEN TEETH TIPS SEEN ON  EXPDI 29
C                  SCHLIEREN PHOTOGRAPH (CM.)                 EXPDI 30
C      U(AND UIN) - FLAME SPEED (CM./SEC)                   EXPDI 31
C      VBFO    - VOLUME PER MOLE OF FUEL (CC./GRAM-MOLE)      EXPDI 32
C      VBM     - VOLUME PER MOLE OF MIXTURE (CC./GRAM-MOLE)    EXPDI 33
C      WF      - FUEL FLOW (GRAM-MOLE/SEC.)                  EXPDI 34
C      WX      - OXIDANT FLOW (GRAM-MOLE/SEC.)                EXPDI 35
C      YOX    - MOLE FRACTION OXYGEN IN OXIDENT              EXPDI 36
C      YOX    - MOLE FRACTION OXYGEN IN OXIDENT              EXPDI 37
C      YOX    - MOLE FRACTION OXYGEN IN OXIDENT              EXPDI 38
C      YOX    - MOLE FRACTION OXYGEN IN OXIDENT              EXPDI 39
C      YOX    - MOLE FRACTION OXYGEN IN OXIDENT              EXPDI 40
SUBROUTINE EXPD1(NRUN,IC1,OFSR,YOX,VBFO,VBM,IPN,O,U,KODE,TEETH,
1 NRUNT 1
COMMON INT,DEC,IC1,J1,J2,J3,NIN,NEX
DIMENSION INT(10),DEC(10)
DIMENSION AI(100),OI(100),DAI(100),H(100),IM(100),FMI(15),
1 OI(15),OF0(15),QMI(15),QXO(15),UM(15)
1 WRITE_OUTPUT TAPE 3, 1010
1 EXPDI 41
1 EXPDI 42
1 EXPDI 43
1 EXPDI 44
1 EXPDI 45
1 EXPDI 46
1 EXPDI 47
1 EXPDI 48
1 EXPDI 49
1 EXPDI 50
1 EXPDI 51
1 EXPDI 52
1 EXPDI 53
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1 EXPDI 90
1 EXPDI 91
1 EXPDI 92
1 EXPDI 93
1 EXPDI 94
1 EXPDI 95
1 EXPDI 96
1 EXPDI 97
1 EXPDI 98
1 EXPDI 99
1 EXPDI 100
1 EXPDI 101
1 EXPDI 102
1 EXPDI 103
1 EXPDI 104
1 EXPDI 105
1 EXPDI 106
C      TEST FOR MORE THAN ONE HUNDRED MEASUREMENTS
C      IF(IPK=100)19,19,20
19 DO 20 K=1,IRK
19   HIK=TEETH*FLOAT(I(HIK)-1)
20   DIK=DAIK*SF
C      CALCULATION OF PEAK HEIGHT IN CM.
C      H(IPK)=HPKA*SF
C      DIIPK=0.0
C      JPK1=1
C      PRINTOUT OF FLAME FRONT DIMENSIONS
C      TEST FOR MORE THAN TEN MEASUREMENTS
C      IF(IPK>10) 24,26,21
21 DO 23 JPK=10,IPK,10
21   IF(L=48)230,230,231
231 WRITE_OUTPUT TAPE 3, 1020
L=0

```

## SUBROUTINE EXPD1

(CONTINUED)

## EXPERIMENTAL FLAME SPEED DATA REDUCTION

```

C PRINTOUT FOR GROUPS OF TEN MEASUREMENTS
C
230 WRITE_OUTPUT TAPE 3, 10121, N = (IHK), K= JPK1, JPK 3 EXPD1 107
C
9 WRITE_OUTPUT TAPE 3, 1013, (IAIK), K= JPK1 , JPK 1 EXPD1 108
C
9 WRITE_OUTPUT TAPE 3, 1014, (IHK) ,K= JPK1 , JPK 1 EXPD1 109
C
9 WRITE_OUTPUT TAPE 3, 1015, (IAIK) ,K= JPK1 , JPK 1 EXPD1 110
C
9 JPK1 = JPK + 1 EXPD1 111
C
23 L = L + 8 EXPD1 112
C
24 JRK = IPK-1 EXPD1 113
C
IF(L=48)25,25,241 EXPD1 114
C
261 WRITE_OUTPUT TAPE 3, 1020 EXPD1 115
L=0 EXPD1 116
C
C PRINTOUT FOR LESS THAN TEN MEASUREMENTS
C
25 WRITE_OUTPUT TAPE 3, 10121, N = (IHK), K= JPK1, JPK 1 EXPD1 117
C
9 WRITE_OUTPUT TAPE 3, 1013, (IAIK), K= JPK1 , JPK 1 EXPD1 118
C
9 WRITE_OUTPUT TAPE 3, 1014, (IHK) ,K= JPK1 , JPK 1 EXPD1 119
C
9 WRITE_OUTPUT TAPE 3, 1015, (IAIK) ,K= JPK1 , JPK 1 EXPD1 120
C
9 JPK1 = JPK + 1 EXPD1 121
C
23 L = L + 8 EXPD1 122
C
24 JRK = IPK-1 EXPD1 123
C
IF(L=48)25,25,241 EXPD1 124
C
261 WRITE_OUTPUT TAPE 3, 1020 EXPD1 125
L=0 EXPD1 126
C
C RUN NUMBER CONSISTENCY CHECK
C
27 IF (INRUN - NRUNT) 30,31,30 EXPD1 127
30 KODE = 1 EXPD1 128
NRUNT = NRUNT EXPD1 129
GO TO 100 EXPD1 130
C
C CONTROL INTEGER CHECK
C
31 IF ((ICL - ICANT) 30,33,30 EXPD1 131
C
C CALCULATION OF OXIDANT AND FUEL FLOW
C
32 WK = QXQIN1/22414.0 EXPD1 132
WF = QFOIN1/VBFO EXPD1 133
QMIN1 = (WF + WK) * VBM / (1.0 - EM1LN) EXPD1 134
C
C CALCULATION OF EQUIVALENCE_RATIO
C
33 QIN1 = WF*QFSW/12.0*WX*YOK EXPD1 135
IRK = IPK-1 EXPD1 136
C
C CALCULATION OF CONE_AREA
C
34 AR = 0.0 EXPD1 137
DO 40 K=1, INK EXPD1 138
DELS = SQRT((IHK(K)) - (IHK))**2 + ((D(K)) - (D(K+1)))**2) EXPD1 139
40 AR = AR + (D(K) + D(K+1))/DELS EXPD1 140
AIN1 = 3.570796*AR EXPD1 141
C
C CALCULATION OF FLAME SPEED
C
35 UIN1 = QMIN1/AIN1 EXPD1 142
100 CONTINUE EXPD1 143
IF(L+LM=56)101,101,102 EXPD1 144
102 WRITE_OUTPUT TAPE 3, 1018 EXPD1 145
L = 0 EXPD1 146
C
C PRINTOUT OF FLAME SPEED
C
101 WRITE_OUTPUT TAPE 3, 1016 EXPD1 147
DO 110 N=1,1PN EXPD1 148
110 WRITE_OUTPUT TAPE 3, 1017 EXPD1 149
N = NRUNT EXPD1 150
NRUNT = IRUNT EXPD1 151
120 RETURN EXPD1 152
C
C DIAGNOSTIC - UNACCEPTABLE CARD ORDER
C
200 NEX = 2 EXPD1 153
WRITE_OUTPUT TAPE 3, 3000, IC, J11 EXPD1 154
KODE = 1 EXPD1 155
GO TO 120 EXPD1 156
C
C FORMAT STATEMENTS
C
1010 FORMAT 9 (1HO, 10X, 22HFLAME FRONT DIMENSIONS / 1HO, 4H SET. ) EXPD1 157
10121 FORMAT 9 (1HO, 14, 2X, 19HSTATION (MEASURED) ,4X, 1019 ) EXPD1 158
1013 FORMAT 9 (1H, 6X, 19HDIAMETER (MEASURED), 4X, 10F 9.3 ) EXPD1 159
1014 FORMAT 9 (1H, 6X, 14HHEIGHT (CM.), 9X, 10F 9.3 ) EXPD1 160
1015 FORMAT 9 (1H, 6X, 14HDIAMETER (CM.) , 9X, 10F 9.5 ) EXPD1 161
10151 FORMAT 9 (1H , 6X, 12HSCALE FACTOR 3X, F 10.5 ) EXPD1 162
1016 FORMAT 9 (1HO, 4H SET, 7X, 9HFUEL FLOW , 4X, 12HOXIDANT FLOW , 3X, 13HMOLE FRACTION , 5X, 11HVOLUME FLOW , 7X, 9HCONE AREA , 2 5X, 11HFLAME SPEED , 5X, 11HEQUIVALENCE , 3 1M, 1LIX, 9H(CC./SEC), 4X, 9H(CC./SEC), 4X, 9HINHIBITOR , 4 8X, 9H(CC./SEC), 8X, 9HISO, CM.1 , 6X, 9H(CN./SEC) , 5 9X , 5HRATIO ) EXPD1 163

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## SUBROUTINE EXPD1

(CONTINUED)

## EXPERIMENTAL FLAME SPEED DATA REDUCTION

1017 FORMAT		EXPD1	213
9 (1H , 14, 6X,F10.5,6X,F10.5,6X,F10.5,6X,F10.5,6X,F10.5,		EXPD1	214
1,6X,F10.5)		EXPD1	215
1018 FORMAT		EXPD1	216
9 (1H1)		EXPD1	217
1020 FORMAT		EXPD1	218
9 (1H1, 10X,22HFLAME FRONT DIMENSIONS /1HO ,4H RUN )		EXPD1	219
3000 FORMAT( 1HO, 25X, 41HDATA CARD ORDER INCORRECT - CARD NUMBER		EXPD1	220
1, 14, 5X, 12HRUN NUMBER 15 )		EXPD1	221
EHD		EXPD1	222

## SUBROUTINE EXPD3

## EXPERIMENTAL FLAME SPEED DATA REDUCTION

```

C EXPD3 EXPD3 SUBROUTINE MOD1 SEPT 8, 1962 MRC DAYTON
C
C Nomenclature
C
C AR - CUMULATIVE CONE AREA = $\pi$ /4
C A(K) - TOTAL CONE AREA (SQ. CM.)
C D(K) - CONE DIAMETER AT ABOVE ELEVATION (CM.)
C DA(K) - MEASURED DIAMETER AT ABOVE ELEVATION
C DELS - INCREMENT SLANT HEIGHT (CM.)
C ELA - REFERENCE LENGTH MEASURED IN UNITS OF DA(K)
C ELCM - REFERENCE LENGTH MEASURED IN CM.
C FM(N) - MOLE FRACTION OF INHIBITOR IN MIXTURE
C H(K) - ELEVATION ABOVE BURNER TOP (CM.)
C HPKA - MEASURED PEAK HEIGHT
C ICANT - OPTION CONTROL INTEGER CHECK
C IH(K) - MEASURED ELEVATION ABOVE BURNER TOP
C IPK - TOTAL NUMBER OF CONE MEASUREMENTS
C IPN - NUMBER OF EXPERIMENTS
C IRK - NUMBER OF DIAMETER MEASUREMENTS PER RUN
C JPK, JPK1, N, K - COUNTING INTEGERS
C KODE - SIGNAL INTEGER FOR ACCEPTABLE DATA
C NRUN - RUN NUMBER OF DATA GROUP
C NRUNT - RUN NUMBER CHECK
C O AND O(N) - EQUIVALENCE RATIO
C DFSR - ATOMS OF OXYGEN TO COMPLETELY OXIDIZE ONE
C MOLECULE OF FUEL
C OFD(N) - FUEL FLOW (CC./SEC AT VBFO MOLAL VOLUME)
C OM(N) - VOLUME FLOW OF MIXTURE (CC./SEC AT ACTUAL
C TEMPERATURE AND PRESSURE)
C OXO(N) - OXIDANT FLOW (CC./SEC AT 0 DEG. C., 760 MM. HG)
C SF - SCALE FACTOR (CM./UNITS OF DA(K))
C TEETH - ACTUAL DISTANCE BETWEEN TEETH TIPS SEEN ON
C SCHLIEREN PHOTOGRAPH (CM.)
C U AND V(N) - FLAME SPEED (CM./SEC.)
C VBFO - VOLUME PER MOLE OF FUEL (CC./GRAM-MOLE)
C VBM - VOLUME PER MOLE OF MIXTURE (CC./GRAM-MOLE)
C WF - FUEL FLOW (GRAM-MOLE/SEC.)
C WO - OXIDANT FLOW (GRAM-MOLE/SEC.)
C YOX - MOLE FRACTION OXYGEN IN OXIDENT
C
C SUBROUTINE EXPD3(NRUN, ICTL, DFSR, YOX, VBFO, VBM, IPN, O, U, KODE, TEETH,
C NRUNT)
C COMMON INT, DEC, IC, J1, J2, J3, NIN, NEX
C DIMENSION A(100), D(100), DA(100), HI(100), IH(100), FM(15)
C D(115), O(115), OM(115), OXO(115), U(15)
C
C WRITE OUTPUT TAPE 3, 1010
C
C L=0
C KODE = 3
C DO 100 N=1,IPN
C
C 10 CALL INPUT
C
C NEX = NRUN
C
C IF(NEX .EQ. 200, 11, 200
C 11 NUMCON = 1C .. 4000
C IF(NUMCON ) 13, 12, 13
C
C 12 O CARD ASSIGNMENTS
C
C 12 NRUNT = J11
C ICANT = INT(1)
C IRK = INT(2)
C OFD(1) = DEC(1)
C OXO(1) = DEC(2)
C FM(1) = DEC(3)
C HPKA = DEC(4)
C ELCM = DEC(5)
C ELA = DEC(6)
C GO TO 10
C
C 13 IF(NRUNT - J11) 200, 141, 200
C 14 LIMIT = 10*NUMCON
C 15 IGO = LIMIT - 9
C 16 IF(LIMIT - IRK ) 142, 142, 140
C 140 LIMIT = IRK
C 142 M = 0
C
C 143 M = 100, LIMIT
C
C M = M + 1
C 144 IH(K) = INT(M)
C 145 DA(K) = DEC(M)
C
C 146 NRUN = NRUN + N - 1
C
C 147 TEETH(14,15,14
C
C 15 TEETH = 0.2
C 14 SF = ELCM / ELA
C
C 16 IPK = IRK + 1
C
C TEST FOR MORE THAN ONE HUNDRED MEASUREMENTS
C
C 17 IF(IPK>100) 19, 19, 30
C 19 DO 20 K = 1, IRK
C 20 H(K) = TEETH * FLOAT(IH(K)-1)
C
C 20 D(K) = DA(K)*SF
C
C CALCULATION OF PEAK HEIGHT IN CM.
C
C 21 HI(IPK) = HPKA * SF
C 22 D(IPK) = 0.0
C 23 JPK1 = 1
C
C PRINTOUT OF FLAME FRONT DIMENSIONS
C
C TEST FOR MORE THAN TEN MEASUREMENTS
C
C 24 IF(IPK>10) 24, 24, 21
C 25 DO 23 JPK=1,IPK,10
C 26 IF(I=48) 230, 230, 231
C 27 231 WRITE OUTPUT TAPE 3, 1020

```

## SUBROUTINE EXPD3

(CONTINUED)

## EXPERIMENTAL FLAME SPEED DATA REDUCTION

```

L=0
C PRINTOUT FOR GROUPS OF TEN MEASUREMENTS
C
230 WRITE OUTPUT TAPE 3, 10121
  9 IRUN, (IH(K), K= JPK1, JPK )
  WRITE OUTPUT TAPE 3, 10131
  9 (DAIK), K= JPK1, JPK 1
  WRITE OUTPUT TAPE 3, 10141
  9 (H(K)), K= JPK1, JPK 1
  WRITE OUTPUT TAPE 3, 10151
  9 (DK(K), K= JPK1, JPK )
  JPK1 = JPK + 1
23 L= L+ 8
24 IF(L=48)25,25,241
241 WRITE OUTPUT TAPE 3, 1020
  L=0.
C PRINTOUT FOR LESS THAN TEN MEASUREMENTS
C
25 WRITE OUTPUT TAPE 3, 1012
  9 IRUN, HPKA, (IH(K), K= JPK1, IRK )
  WRITE OUTPUT TAPE 3, 1013
  9 (DAIK), K= JPK1, IRK 1
  WRITE OUTPUT TAPE 3, 1014
  9 (H(K), K= JPK1, IRK 1
  WRITE OUTPUT TAPE 3, 1015
  9 (DK(K), K= JPK1, IRK )
  WRITE OUTPUT TAPE 3, 10151
  9 ELCM, ELA
  L= L+10.
C RUN NUMBER CONSISTENCY CHECK
C
30 IF (IRUN.= NRUN) 30,31,30
  30 KODE = 1
  IRUNT = NRUNT
  GO TO 100
C CONTROL INTEGER CHECK
C
31 IF (IC1L < ICANT) 30,35,30
C CALCULATION OF OXIDANT AND FUEL FLOW
C
35 MX = QOIN(1)/22414.0
  WF = QFQIN(1)/VBFO
  QH(N) = (WF + WX) * VBM / (1.0 - FM(N))
C CALCULATION OF EQUIVALENCE RATIO
C
36 DIN = WF*QFSR/(2.0*MX*VOX)
C CALCULATION OF CONE AREA
C
37 AR = 0.0
  DO 40 K = 1, IRK
  DELS = SQRT((H(K+1) - H(K))**2 + (D(K) - D(K+1))**2)
  40 AR = AR + (DK(K) + D(K+1))*DELS
  AIN = 1.570796*AR
C CALCULATION OF FLAME SPEED
C
38 UIN = QH(N)/AIN
  100 CONTINUE
  IF(L+IPN = 56) 101,101,102
  102 WRITE OUTPUT TAPE 3, 1018
  L=0
C PRINTOUT OF FLAME SPEED
C
101 WRITE OUTPUT TAPE 3, 1016
  DO 110 N=1,IPN
  IRUN = NRUN - 1 + N
110 WRITE OUTPUT TAPE 3, 1017,
  9 IRUN, QEO(N), QXO(N), FM(N), QH(N), AIN, UIN, DIN
  NRUNT = IRUN
120 RETURN
C DIAGNOSTIC - UNACCEPTABLE CARD ORDER
C
200 NEX = 2
  WRITE OUTPUT TAPE 3, 3000, IC, 311
  KODE = 1
  GO TO 120
C FORMAT STATEMENTS
C
1010 FORMAT
  9 (1H0, 10X, 2MHFLAME FRONT DIMENSIONS /1H0, 4H RUN )
1012 FORMAT
  9 (1H0, 14. 2X, 2MHPEAK HEIGHT (MEASURED UNITS) FB.2 /
  1 1H , 6X, 19HSTATION (MEASURED), 4X, 1019)
10121 FORMAT
  9 (1H0, 14. 2X, 19HSTATION (MEASURED), 4X, 1019)
1013 FORMAT
  9 (1H , 6X, 19HDIAMETER (MEASURED), 4X, 10F 9.3 )
1014 FORMAT
  9 (1H , 6X, 14MHHEIGHT (CM.) , 9X, 10F 9.5 )
1015 FORMAT
  9 (1H , 6X, 14HDIAMETER (CM.) , 4X, 10F 9.5 )
10151 FORMAT
  9 (1H , 6X, 26MACTUAL LENGTH OF REFERENCE 3X,10.5,3X, 3HCM,
  1 1X, 2X, 2MHMEASURED LENGTH OF REFERENCE 3X,10.5,3H UNITS )
1016 FORMAT
  9 (1H0, 4H RUN, TX, 4H FUEL FLOW , 4X, 12HOXIDANT FLOW.. 3X)

```

## SUBROUTINE EXPD3

(CONTINUED)

## EXPERIMENTAL FLAME SPEED DATA REDUCTION

1 I3MHOLE FRACTION , SX, 11MVOLUME FLOW , TX, 19CONE AREA	EXP03	213
2 SX, 11MFLAME SPEED , SX, 11MEQUIVALENCE	EXP03	214
3 1M , 11X, 19LCC./SEC), 6X, 19LG.(/SEC) , 6X, 19INHIBITOR	EXP03	215
4 6X , 19LCC./SEC), 6X, 19LG.(/SEC) , 6X, 19INHIBITOR	EXP03	216
5 9X , 19LCC./SEC), 6X, 19LG.(/SEC) , 6X, 19INHIBITOR	EXP03	217
1017 FORMAT	EXP03	218
9 (1H , 14, 6X,F10.5,6X,F10.5,6X,F10.5,6X,F10.5,6X,F10.5,6X)	EXP03	219
1 6X,F10.5)	EXP03	220
1018 FORMAT	EXP03	221
9 (1H)	EXP03	222
1020 FORMAT	EXP03	223
9 (1H), 10X, 22MFLAME FRONT DIMENSIONS /1HO , 4H RUN)	EXP03	224
3000 FORMAT(1HO, 25X, 4)HO DATA CARD ORDER, INCORRECT - CARD NUMBER	EXP03	225
1 14, SX, 12HRUN NUMBER (S )	EXP03	226
END	EXP03	227

## SUBROUTINE MAXM

## MAXIMUM FLAME SPEED DETERMINATION

```

CMAXH SUBROUTINE MAXM FOR ROUTINE 2010 FEB 28 1962 MAC - DAYTON      MAXM  1
C                                              NOMENCLATURE                      MAXM  2
C                                              MAXM  3
C                                              MAXM  4
C A(K)   - COEFFICIENTS OF FITTED EQUATION                         MAXM  5
C ARG    - ARGUMENT OF QUADRATIC SQUARE ROOT                          MAXM  6
C G(J,K) - SUM OF SQUARES AND CROSS PRODUCTS OF THE                MAXM  7
C          X(M,K) MATRIX                                         MAXM  8
C IPN    - NUMBER OF DATA POINTS                                     MAXM  9
C J, K, L, N - INDICES                                             MAXM 10
C K9     - SIGNAL FLAG FOR SEQUENCE OF CALCULATIONS                 MAXM 11
C KODE   - SIGNAL INTEGER FOR ACCEPTABLE DATA                      MAXM 12
C MAXON  - SWITCH TO BYPASS MAXM SUBROUTINE                         MAXM 13
C          (ANY NON-ZERO VALUE BYPASSES SUBROUTINE)                  MAXM 14
C NCF    - NUMBER OF COEFFICIENTS                                    MAXM 15
C O(N)   - EQUIVALENCE RATIO                                         MAXM 16
C OH    - LARGEST EQUIVALENCE RATIO IN SET                           MAXM 17
C OINF   - EQUIVALENCE RATIO AT INFLECTION POINT OF CUBIC...     MAXM 18
C          CUBE                                           MAXM 19
C OL    - SMALLEST EQUIVALENCE RATIO IN SET                          MAXM 20
C OMX   - EQUIVALENCE RATIO AT MAXIMUM FLAME VELOCITY               MAXM 21
C STD5   - MAXIMUM ALLOWABLE STANDARD DEVIATION OF U VS           MAXM 22
C          U CURVE FOR ADDITION TO TAPE                            MAXM 23
C SUM   - SUM OF THE SQUARES OF THE DEVIATIONS                     MAXM 24
C U(M)  - FLAME SPEED (CM./SEC)                                      MAXM 25
C UD(M) - DEVIATION BETWEEN MEASURED AND PREDICTED                 MAXM 26
C          FLAME SPEED (CM./SEC)                                     MAXM 27
C UDP(N) - PERCENT DEVIATION BETWEEN MEASURED AND                 MAXM 28
C          PREDICTED FLAME SPEED                               MAXM 29
C UMX   - MAXIMUM FLAME SPEED (CM./SEC)                            MAXM 30
C UP(N) - PREDICTED FLAME SPEED (CM./SEC)                           MAXM 31
C USID  - STANDARD DEVIATION OF FLAME SPEED (CM./SEC)             MAXM 32
C USTOC - FLAME SPEED AT STOICHIOMETRIC CONDITIONS              MAXM 33
C          (CM./SEC)                                         MAXM 34
C X(M,K) - INDEPENDENT VARIABLES
C          SUBROUTINE MAXM, IPN, O, U, OMX, UMX, USTOC, KODE, STD5, MAXM 35
C          IEXPD, MAXON, NRUN, I
C 1      COMMON INT, DEC, (J1, J2, J3, NIN, NEX...)                   MAXM 36
C          DIMENSION INT(10), DEC(10)                                 MAXM 37
C          DIMENSION A(10), G(10,11), O(10), U(10), UDP(10), UP(10), X(10,11) MAXM 38
C          1)
C          KODE = 0,                                                 MAXM 39
C          IF(MAXON) 500, 20, 500                                     MAXM 40
C 20 WRITE OUTPUT TAPE 3, 1001
C          IF (IPN = 2) 500, 500, 25
C 25 OL = O(L)
C          OH = OL
C          DO 30 N=1,IPN
C          OL = MINIFOL,O(N))
C          OH = MAXIFOH,O(N)).
C 30
C          C FORMATION OF COEFFICIENT MATRIX
C          X(1,1) = 1.0
C          X(1,2) = O(N)
C          X(1,3) = O(N)*2
C          X(1,4) = O(N)*3
C 30. X(1,5) = U(N)
C 30.
C          C TEST FOR MORE THAN FOUR DATA POINTS
C          IF (IPN = 4) 150,40,50
C 40
C          C ATTEMPT TO FIT FOUR DATA POINTS TO A FOUR CONSTANT EQUATION
C          C SOLUTION OF FOUR EQUATIONS IN FOUR UNKNOWNNS
C          C 40 CALL CROUT (4,X,A)
C          C TEST FOR UNSUCCESSFUL SOLUTION
C          C IF (.SENSE LIGHT 3) 41, 70
C          C PRINTOUT OF UNSUCCESSFUL FIT
C          C 41 WRITE OUTPUT TAPE 3, 1010
C          C          WRITE OUTPUT TAPE 3, 1011,
C          C          ((X(K,L),L=1,5),K=1,4)
C          C GO TO 200
C          C ATTEMPT TO FIT FOUR OR MORE DATA POINTS TO A FOUR CONSTANT
C          C EQUATION
C          C 50,DO,60,J=1,4
C          DO 60 K=1,5
C          GL,J,K) = 0.0
C          DO 60 N=1,IPN
C          C GENERATION OF FOUR REGRESSION EQUATIONS
C          C 60 G(J,K) = G(J,K) + X(M,J)*X(M,K)
C          C SOLUTION OF FOUR REGRESSION EQUATIONS IN FOUR UNKNOWNNS
C          C 61 CALL CROUT (4,G,A)
C          C IF (.SENSE LIGHT 3) 61, 70
C          C PRINTOUT OF UNSUCCESSFUL FIT
C          C 61 WRITE OUTPUT TAPE 3, 1010
C          C          WRITE OUTPUT TAPE 3, 1011,
C          C          ((G(K,L),L=1,5),K=1,9)
C          C GO TO 200
C          C OPERATIONS ON FOUR OR MORE DATA POINTS
C          C

```

## SUBROUTINE MAXM

(CONTINUED)

## MAXIMUM FLAME SPEED DETERMINATION

```

70 NCF = 4... MAXM 107
K9 = 1 MAXM 108
IF DIVIDE CHECK 71, 71 MAXM 109
71 DMX = 0.0 MAXM 110
DMX = 0.0 MAXM 111
DINF = -A(3)/13.0*A(4) MAXM 112
IF DIVIDE CHECK 310, 72 MAXM 113
72 K9 = 2 MAXM 114
ARG = 1.0 - 3.0*A(2)*A(4)/A(3)**2 MAXM 115
IF DIVIDE CHECK 310, 80 MAXM 116
C MAXM 117
C TEST FOR SQUARE ROOT OF NEGATIVE NUMBER MAXM 118
C MAXM 119
80 IF (ARG) 310, 310, 85 MAXM 120
85 K9 = 3 MAXM 121
C DETERMINATION OF EQUIVALENCE RATIO AT MAXIMUM FLAME SPEED MAXM 122
C MAXM 123
OMX = DINF*(1.0 + SIGNF(SORTF(ARG), A(3))) MAXM 124
MAXM 125
MAXM 126
C TEST TO SEE IF EQUIVALENCE RATIO AT MAXIMUM FLAME SPEED IS WITHIN MAXM 127
C DATA RANGE MAXM 128
C MAXM 129
IF (OMX - DMX) 90, 90, 300 MAXM 130
90 IF (OL - OMX) 95, 95, 300 MAXM 131
95 K9 = 4 MAXM 132
DINF = DINF + (1.0 - SIGNF(SORTF(ARG), A(3))) MAXM 133
MAXM 134
C TEST FOR MINIMUM POINT IN DATA RANGE MAXM 135
C MAXM 136
IF (OMIN - DMX) 100, 110, 110 MAXM 137
100 IF (OL - OMIN) 300, 110, 110 MAXM 138
110 K9 = 7 MAXM 139
GO TO 300 MAXM 140
C MAXM 141
C END OF OPERATION ON CUBIC FIT MAXM 142
C MAXM 143
C ATTEMPT TO FIT THREE DATA POINTS TO A THREE CONSTANT EQUATION MAXM 144
C MAXM 145
150 DO 160 N=1, IPN MAXM 146
160 X(N,A) = U(N) MAXM 147
CALL CRUT (3,X,A) MAXM 148
IFI SENSE LIGHT 3, 161, 230 MAXM 149
MAXM 150
C PRINTOUT OF UNSUCCESSFUL FIT MAXM 151
C MAXM 152
161 WRITE OUTPUT TAPE 3, 1012 MAXM 153
WRITE OUTPUT TAPE 3, 1013 MAXM 154
9 ((X(K,L),L=1,4),K=1,3) MAXM 155
MAXM 156
GO TO 500 MAXM 157
C ATTEMPT TO FIT FOUR OR MORE DATA POINTS TO A THREE CONSTANT MAXM 158
C EQUATION MAXM 159
C MAXM 160
200 DO 210 N=1, IPN MAXM 161
210 X(N,A) = U(N) MAXM 162
DO 220 J=1,3 MAXM 163
..DU,220,K=1,4 MAXM 164
..G(J,K) = 0.0 MAXM 165
DO,220,N=1,IPN MAXM 166
C GENERATION OF THREE REGRESSION EQUATIONS MAXM 167
MAXM 168
220,G1J,K1 = G1J,K1 + X(N,J)*X(N,K) MAXM 169
MAXM 170
C SOLUTION OF THREE EQUATIONS IN THREE UNKNOWN MAXM 171
MAXM 172
C CALL CRUT (3,G,A) MAXM 173
MAXM 174
C TEST FOR UNSUCCESSFUL SOLUTION MAXM 175
MAXM 176
IFI SENSE LIGHT 3, 1, 221, 230 MAXM 177
MAXM 178
C PRINTOUT OF UNSUCCESSFUL FIT MAXM 179
MAXM 180
C 222, WRITE OUTPUT TAPE 3, 1012 MAXM 181
WRITE OUTPUT TAPE 3, 1013 MAXM 182
9 ((G(K,L),L=1,4),K=1,3) MAXM 183
MAXM 184
GO TO 500 MAXM 185
MAXM 186
C OPERATIONS ON THREE OR MORE DATA POINTS MAXM 187
C MAXM 188
230 NCF = 3 MAXM 189
K9 = 2 MAXM 190
A(4) = 0.0 MAXM 191
UMX = 0.0 MAXM 192
DMX = 0.0 MAXM 193
IF (A(3)) 240, 310, 310 MAXM 194
240 K9 = 6 MAXM 195
C DETERMINATION OF EQUIVALENCE RATIO AT MAXIMUM FLAME SPEED MAXM 196
MAXM 197
MAXM 198
DMX = -A(2)/(2.0*A(3)) MAXM 199
MAXM 200
C TEST TO SEE IF EQUIVALENCE RATIO AT MAXIMUM FLAME SPEED IS WITHIN MAXM 201
C .. DATA RANGE MAXM 202
C MAXM 203
IF (OMX - DMX) 250, 250, 300 MAXM 204
250 IF (OL - OMX) 260, 260, 300 MAXM 205
MAXM 206
C END OF OPERATION ON PARABOLIC FIT MAXM 207
C MAXM 208
C OPERATION ON DATA AFTER SUCCESSFUL FIT MAXM 209
MAXM 210
260 K9 = 7 MAXM 211
MAXM 212

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## SUBROUTINE MAXH

(CONTINUED)

## MAXIMUM FLAME SPEED DETERMINATION

```

C      CALCULATION OF MAXIMUM FLAME SPEED          MAXH  213
C      300_UMX = A(1) + OMX*(A(2) + OMX*(A(3) + OMX*A(4)))    MAXH  214
C      MAXH  215
C      MAXH  216
C      MAXH  217
C      310 USTOC = A(1) + A(2) + A(3) + A(4)    MAXH  218
C      SUM = 0.0    MAXH  219
C      DO_320_N=1,_IPN    MAXH  220
C      UP(N) = A(1) + O(N)*(A(2) + O(N)*(A(3) + O(N)*A(4)))    MAXH  221
C      MAXH  222
C      MAXH  223
C      COMPARISON OF PREDICTED VS. MEASURED EQUIVALENCE RATIOS    MAXH  224
C      MAXH  225
C      UDIN = U(N) - UP(N)    MAXH  226
C      MAXH  227
C      CALCULATION OF THE PERCENT ERROR OF THE DEVIATION    MAXH  228
C      MAXH  229
C      UDP(N) = 100.0*UD(N)/UP(N)    MAXH  230
C      MAXH  231
C      SUMMATION OF THE SQUARE OF THE DEVIATIONS    MAXH  232
C      MAXH  233
C      320 SUM = SUM + UD(N)**2    MAXH  234
C      IF (IPN - NCF) 330,330,340    MAXH  235
C      330 USTD = 0.0    MAXH  236
C      GO TO 350    MAXH  237
C      MAXH  238
C      MAXH  239
C      CALCULATION OF STANDARD DEVIATION OF FLAME SPEED    MAXH  240
C      MAXH  241
C      340 USTD = SQRT(SUM/FLOAT(IPN-NCF))    MAXH  242
C      350 WRITE OUTPUT TAPE 3, 1014    MAXH  243
C      WRITE OUTPUT TAPE 3, 1015    MAXH  244
C      WRITE OUTPUT TAPE 3, 1016    MAXH  245
C      9 (A(K),K=1,4),USTD,OMX,UMX    MAXH  246
C      IF (K9 = 1) 351,352,351    MAXH  247
C      351 WRITE OUTPUT TAPE 3, 10171    MAXH  248
C      DO 354_N=1,_IPN    MAXH  249
C      ITRUN = NRUN + N - 1    MAXH  250
C      354 WRITE OUTPUT TAPE 3, 1018    MAXH  251
C      9 (JRUN, OINI, UINI, UPINI, UDINI, UDPINI)    MAXH  252
C      GO TO 353    MAXH  253
C      352 WRITE OUTPUT TAPE 3, 1017    MAXH  254
C      DO 352_N = 1, IPN    MAXH  255
C      3521 WRITE OUTPUT TAPE 3, 1018    MAXH  256
C      9 (N, OINI, UINI, UPINI, UDINI, UDPINI)    MAXH  257
C      353 IF (K9=4) 360,360,370    MAXH  258
C      ERROR PRINT - CUBIC FIT OF CURVE UNSATISFACTORY    MAXH  259
C      360 WRITE OUTPUT TAPE 3, 1019    MAXH  260
C      GO TO (361,362,363,364), K9    MAXH  261
C      MAXH  262
C      DIAGNOSTIC - PARABOLIC FIT INDICATED, A3 SHALL OR ZERO    MAXH  263
C      MAXH  264
C      MAXH  265
C      361 WRITE OUTPUT TAPE 3, 1020    MAXH  266
C      GO TO 200    MAXH  267
C      MAXH  268
C      ERROR PRINT - NO MAXIMUM    MAXH  269
C      MAXH  270
C      362 WRITE OUTPUT TAPE 3, 1021    MAXH  271
C      GO TO 200    MAXH  272
C      MAXH  273
C      ERROR PRINT - MAXIMUM OUTSIDE DATA RANGE    MAXH  274
C      MAXH  275
C      363 WRITE OUTPUT TAPE 3, 1022    MAXH  276
C      GO TO 200    MAXH  277
C      MAXH  278
C      ERROR PRINT - MINIMUM POINT IN DATA RANGE    MAXH  279
C      MAXH  280
C      364 WRITE OUTPUT TAPE 3, 1023    MAXH  281
C      GO TO 200    MAXH  282
C      370 IF (K9 = 7) 371,380,500    MAXH  283
C      MAXH  284
C      ERROR PRINT - PARABOLIC FIT OF CURVE UNSATISFACTORY    MAXH  285
C      MAXH  286
C      371 WRITE OUTPUT TAPE 3, 1024    MAXH  287
C      IF (K9 = 6) 372,373,500    MAXH  288
C      372 WRITE OUTPUT TAPE 3, 1021    MAXH  289
C      GO TO 500    MAXH  290
C      373 WRITE OUTPUT TAPE 3, 1022    MAXH  291
C      GO TO 500    MAXH  292
C      380 IF (USTD) 381,381,382    MAXH  293
C      381 STD5 = 1.0    MAXH  294
C      MAXH  295
C      TEST TO SEE IF STANDARD DEVIATION WITHIN SPECIFIED RANGE    MAXH  296
C      MAXH  297
C      382 IF (USTD - STD5) 400,400,383    MAXH  298
C      MAXH  299
C      ERROR PRINT - STANDARD DEVIATION TOO HIGH    MAXH  300
C      MAXH  301
C      393 WRITE OUTPUT TAPE 3, 1023    MAXH  302
C      9 STD5    MAXH  303
C      GO TO 500    MAXH  304
C      400 KODE = 3    MAXH  305
C      500 RETURN    MAXH  307
C      MAXH  308
C      MAXH  309
C      1001 FORMAT    MAXH  310
C      9 (1H1)    MAXH  311
C      1011 FORMAT    MAXH  312
C      9 (1H , 10X, E12.5, 10X, E12.5,10X, E12.5,10X,E12.5 )    MAXH  313
C      1012 FORMAT    MAXH  314
C      9 (1H0, 10X, 73HPARABOLIC FIT OF FLAME SPEED CURVE FAILED - MATRIX    MAXH  315
C      1 OF THE COEFFICIENTS IS /    MAXH  316
C      2 1H0, 10X, 12HEQUIV. RATIO , 8X, 16HEQUIV. RATIO **2, 9X,    MAXH  317
C      3 1HFLAME SPEED //)    MAXH  318

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## SUBROUTINE MAXM

(CONTINUED)

## MAXIMUM FLAME SPEED DETERMINATION

1013 FORMAT		MAXM 319
9 (1H, 10X, E12.5, 10X, E12.5, 10X, E12.5, 10X, E12.5)		MAXM 320
1014 FORMAT		MAXM 321
9 (1HO, 10X, 22HFLAME SPEED CURVE DATA )		MAXM 322
1014 FORMAT		MAXM 323
9 (1H, 6X, 414X, 1PE12.4), 5X, 0PF8.4, 8X, F9.5, 9X, F9.4 )		MAXM 324
1017 FORMAT		MAXM 325
9 (1HO, 10X, BHDATA SET ,10X, 11HEQUIVALENCE 10X, BHMEASURED		MAXM 326
1   LIX, BHPREDICTED 10X, BHDEVIATION LIX, 7PERCENT /		MAXM 327
2  1H 3IX, BHRATIO 12X, 11HFLAME SPEED 8X, 11HFLAME SPEED		MAXM 328
3   28X, BHDEVIATION / )		MAXM 329
1017I FORMAT		MAXM 330
9 (1HO, 10X, BH KUM, 10X, 11HEQUIVALENCE 10X, BHMEASURED		MAXM 331
1   LIX, BHPREDICTED 10X, BHDEVIATION LIX, 7PERCENT /		MAXM 332
2  1H 3IX, BHRATIO 12X, 11HFLAME SPEED 8X, 11HFLAME SPEED		MAXM 333
3   28X, BHDEVIATION / )		MAXM 334
1018 FORMAT		MAXM 335
9 (1H, 10X, 18, 10X, F11.4, 10X, F9.4, 10X, F9.4, 10X, F9.4)		MAXM 336
1019 FORMAT		MAXM 337
9 (1HO, 10X, 3SHCUBIC FIT OF CURVE UNSATISFACTORY - )		MAXM 338
1020 FORMAT		MAXM 339
9 (1H+, 47X, 23HPARABOLIC FIT INDICATED )		MAXM 340
1021 FORMAT		MAXM 341
9 (1H+, 47X, 16HNO MAXIMUM FOUND )		MAXM 342
1022 FORMAT		MAXM 343
9 (1H+, 47X, 26HMAXIMUM OUTSIDE DATA RANGE )		MAXM 344
1023 FORMAT		MAXM 345
9 (1H+, 47X, 27HMINIMUM POINT IN DATA RANGE )		MAXM 346
1024 FORMAT		MAXM 347
9 (1HO, 6X, 39HPARABOLIC FIT OF CURVE UNSATISFACTORY - )		MAXM 348
1025 FORMAT		MAXM 349
9 (1HO, 10X, 31HSTANDARD DEVIATION GREATER THAN F6.3 )		MAXM 350
1026 FORMAT		MAXM 351
9 (1HO, 10X, 69HCUBIC FIT OF FLAME SPEED CURVE FAILED - MATRIX OF		MAXM 352
1THE COEFFICIENTS IS .		MAXM 353
2 1HO, 10X 12HEQUIV. RATIO , 8X,16HEQUIV. RATIO +02 , 6X,		MAXM 354
3   16HEQUIV. RATIO +03 , 8X,11HFLAME SPEED / )		MAXM 355
1015 FORMAT		MAXM 356
9 (1HO, 34X, 12HCOEFFICIENTS -30X, 0RHSTANDARD , 4X,		MAXM 357
1   17HEQUIVALENCE RATIO , 6X, 7HMAXIMUM /		MAXM 358
2  1H , 15X, 2H1A1, 15X, 2H2A2, 14X, 2H3A3, 14X, 2H4A4 , 10X,		MAXM 359
3   9HDEVIATION , 3X, 18HAT MAX FLAME SPEED , 3X,		MAXM 360
4   11HFLAME SPEED / )		MAXM 361
END		MAXM 362

## SUBROUTINE TAPE

## MASTER LIBRARY TAPE MODIFICATION

CTAPE	SUBROUTINE TAPE FOR ROUTINE 2018 MARCH 5, 1962 NRC - DAYTON	TAPE	1
C	NOMENCLATURE	TAPE	2
C	A1(1) AND A2(1) - FUEL NAME	TAPE	3
C	ACCL(L,K) - NUMBER OF STRUCTURAL CONTRIBUTORS PER MOLECULE	TAPE	4
C	IN REVISED LIST	TAPE	5
C	AGNL(K), L1(K,1) - CONTRIBUTOR NAMES (FROM CARDS)	TAPE	6
C	D1(K,1) - NUMBER OF STRUCTURAL CONTRIBUTORS PER MOLECULE	TAPE	7
C	BLK - BLANK (USED IN CONTRIBUTOR NAME LIST)	TAPE	8
C	D1(K) - DECIMAL DATA STORAGE	TAPE	9
C	DNMK(K) - DEPENDENT VARIABLE NAME LIST	TAPE	10
C	DU AND TE - FIRST AND SECOND HALVES OF DATE	TAPE	11
C	FGCCJL(J) - NUMBER OF STRUCTURAL CONTRIBUTORS PER MOLECULE	TAPE	12
C	FOR CONTRIBUTOR NUMBER LFGCCN(K)	TAPE	13
C	FGCL(K) - NUMBER OF STRUCTURAL CONTRIBUTORS PER MOLECULE	TAPE	14
C	FOR CONTRIBUTOR NUMBER LFGCCN(K)	TAPE	15
C	FN1 AND FN2 - FIRST AND SECOND HALVES OF FUEL NAME	TAPE	16
C	GNL(J) - CONTRIBUTOR NAME (FROM TAPE)	TAPE	17
C	I,J,K,L - INDICES	TAPE	18
C	IIA(I) - FUEL CLASS NUMBER	TAPE	19
C	LIB(L) - FUEL GROUP NUMBER	TAPE	20
C	LLC(L) - FUEL MEMBER NUMBER	TAPE	21
C	L2(L) - DATA SOURCE NUMBER	TAPE	22
C	LS(L) - EXPERIMENTAL CONDITIONS NUMBER	TAPE	23
C	LA(L) - NUMBER OF STRUCTURAL CONTRIBUTORS CONSIDERED	TAPE	24
C	IADD - NUMBER OF DATA GROUPS ACCEPTABLE FOR WRITING	TAPE	25
C	ICANI - OPTION CONTROL INTEGER CHECK	TAPE	26
C	ICTL - OPTION CONTROL INTEGER	TAPE	27
C	IFNC - FUEL CLASS NUMBER	TAPE	28
C	IFNG - FUEL GROUP NUMBER	TAPE	29
C	IFNM - FUEL MEMBER NUMBER	TAPE	30
C	INDS - DATA SOURCE CODE FOR GROUP SERIAL NUMBER ISFN	TAPE	31
C	INEC - DATA EXPERIMENTAL CONDITIONS CODE FOR GROUP	TAPE	32
C	SERIAL NUMBER ISFN	TAPE	33
C	IPACC - NUMBER OF CONTRIBUTOR COUNT CHANGES FOLLOWING	TAPE	34
C	REMAINDER OF -G- CARD	TAPE	35
C	IPCN - NUMBER OF CONTRIBUTOR NAME CHANGES FOLLOWING	TAPE	36
C	SIX PER -H- CARD	TAPE	37
C	IPGCC - NUMBER OF PAIRS IN CONTRIBUTOR COUNT LIST	TAPE	38
C	FOLLOWING ON TAPE	TAPE	39
C	IPFM - NUMBER OF CARDS FOLLOWING WITH CONTRIBUTOR	TAPE	40
C	COUNT CHANGES I-G- CARDS	TAPE	41
C	IPI - NUMBER OF GROUPS ON TAPE 2 BEFORE ADDITIONS	TAPE	42
C	IPIN - NUMBER OF GROUPS ON TAPE 2 AFTER ADDITIONS	TAPE	43
C	ISFN - DATA GROUP SERIAL NUMBER (FROM TAPE 2)	TAPE	44
C	ITP - CODE INTEGER FOR INITIAL TAPE PREPARATION	TAPE	45
C	J1(K,1) - SPECIES CONTRIBUTOR CODE NUMBER	TAPE	46
C	JGNL(K) - CONTRIBUTOR CODE NUMBER	TAPE	47
C	KI - NUMBER OF STRUCTURAL CONTRIBUTORS CONSIDERED	TAPE	48
C	LACN(L,K) - CONTRIBUTOR CODE NUMBER (FROM CARDS)	TAPE	49
C	LFGCCN(K) - CONTRIBUTOR CODE NUMBER (FROM TAPE)	TAPE	50
C	LFNN(L) - DATA GROUP SERIAL NUMBER (FROM CARDS)	TAPE	51
C	LFNN(L) - NUMBER OF CONTRIBUTOR COUNT CHANGES FOR DATA	TAPE	52
C	GROUP SERIAL NUMBER LFNN(L)	TAPE	53
C	LIPACC(L) - COUNTING INTEGER FOR LINES PRINTED PER PAGE	TAPE	54
C	M - RUN NUMBER CHECK	TAPE	55
C	NRUN - RUN NUMBER OF DATA GROUP	TAPE	56
C	NRUNT - RUN NUMBER CHECK	TAPE	57
C	SUBROUTINE TAPE (NRUN,ICTL,A1,A2,IIA,LIB,LLC,I2,I3,DA,I4,J1,B1,	TAPE	58
1	IADD,DU,TE, LAST)	TAPE	59
C	COMMON INT, DEC, IC, J11, J2, J3, NIN, NEX	TAPE	60
C	DIMENSION INT(10), DEC(10)	TAPE	61
C	DIMENSION A1(20),AZ1(20),B1(100,20),D1(6,20),II1(20),I2(20),I3(20)	TAPE	62
1	,I4(20),J1(100,20),ACCL(20,90),AGNL(50),D1(6),DNM(6),FGCL(90),	TAPE	63
2	FGCJL(200),GNL(200),JGNL(50),LACN(20,90),LFNN(20),LGCCN(90),	TAPE	64
3	LIPACC(20), II1(20), LIB(20), LLC(20)	TAPE	65
C	M = 4	TAPE	66
C	WRITE OUTPUT TAPE 3, 300U	TAPE	67
9	DU,TE	TAPE	68
9	WRITE OUTPUT TAPE 3, 300U	TAPE	69
9	NHNU	TAPE	70
C	REWIND 6	TAPE	71
10	CALL INPUT	TAPE	72
C	NEX = NEX	TAPE	73
C	IF (NEX - 6) 600, 11, 33	TAPE	74
C	F CARD ASSIGNMENTS	TAPE	75
C	11 NRUNT = J11	TAPE	76
C	ICANI = INT(1)	TAPE	77
C	IPFM = INT(2)	TAPE	78
C	IPCN = INT(3)	TAPE	79
C	ITP = INT(4)	TAPE	80
C	LAST = INT(5)	TAPE	81
C	RUN NUMBER CONSISTENCY CHECK	TAPE	82
C	IF (NRUN - NRUNT) 29,21,29	TAPE	83
C	OPTION CONTROL INTEGER CHECK	TAPE	84
C	21 IF (ICANI - ICANI) 29,22,29	TAPE	85
C	TESTS FOR EXECUTABLE CONDITIONS	TAPE	86
C	22 IF (ITP + 7) 25, 28,25	TAPE	87
C	25 IF (IPFM) 26,26,32	TAPE	88
C	TEST FOR GROUPS READY TO BE ADDED	TAPE	89
C	26 IF (IPCN) 27,27,40	TAPE	90
C	27 IF (IADD) 30,30,40	TAPE	91
C	DIAGNOSTIC - INITIAL TAPE PREPARATION	TAPE	92
C	28 WRITE OUTPUT TAPE 3, 300U	TAPE	93
C		TAPE	94
C		TAPE	95
C		TAPE	96
C		TAPE	97
C		TAPE	98
C		TAPE	99
C		TAPE	100
C		TAPE	101
C		TAPE	102
C		TAPE	103
C		TAPE	104
C		TAPE	105
C		TAPE	106

## SUBROUTINE TAPE

(CONTINUED)

## MASTER LIBRARY TAPE MODIFICATION

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GO TO 195                                TAPE 107
C   ERROR PRINT - DATA OUT OF ORDER        TAPE 108
C   TAPE 109
-- 29 WRITE OUTPUT TAPE 3, 3005;          TAPE 110
9      NRUN,NRUNT,ICTL,ICANT             TAPE 111
GO TO 600                                  TAPE 112
C   TAPE 113
C   DIAGNOSTIC - NO ACTION CALLED FOR    TAPE 114
C   TAPE 115
-- 30 WRITE OUTPUT TAPE 3, 3004           TAPE 116
GO TO 495                                  TAPE 117
32 L = 0                                    TAPE 118
321 L = L + 1                            TAPE 119
GO TO 10                                   TAPE 120
C   TAPE 121
C   G CARD ASSIGNMENTS                   TAPE 122
C   TAPE 123
C   33, IFI, NEX - 7, 600, 330, 600       TAPE 124
330 NUMCON = IC - 7000                  TAPE 125
331 LFNNIL = INT(1)                      TAPE 126
332 IPACC = INT(2)                      TAPE 127
GO TO 10                                   TAPE 128
332, IFI, NRUNT - J11, 600, 333, 600     TAPE 129
333 LIMIT = 10*NUNCON                  TAPE 130
100 = LIMIT - 9                         TAPE 131
IF(LIMIT = IPACC) 335, 335, 334         TAPE 132
334 LIMIT = IPACC                      TAPE 133
335 M2= 0                                 TAPE 134
DO 336 K = 100, LIMIT                 TAPE 135
M2, M2+ 1                               TAPE 136
336 L = IPFN 1 321, 40, 40              TAPE 137
LACHN(L,K) = INT(M2)
336 ACCL(L,K) = UEC(M2)                TAPE 138
IFI LIMIT = IPACC) 10, 35, 10           TAPE 139
35 LIPACC(L) = IPACC                  TAPE 140
IFI L = IPFN 1 321, 40, 40              TAPE 141
C   READING OF MASTER TAPE 6             TAPE 142
C   TAPE 143
-- 40 READ INPUT TAPE 6, 2000           TAPE 144
READ INPUT TAPE 6, 2001, IPI            TAPE 145
C   TAPE 146
C   READY SCRATCH TAPE 8               TAPE 147
C   TAPE 148
C   REWIND 8                           TAPE 149
C   TAPE 150
C   TAPE 151
C   COMPUTATIONS FOR ALTERATIONS AND ADDITIONS TO DATA GROUPS ON TAPE TAPE 152
C   TAPE 153
C   DO 90 I=1,IPI                      TAPE 154
C   TAPE 155
C   READ EACH GROUP STORED ON TAPE 6    TAPE 156
C   TAPE 157
C   READ INPUT TAPE 6, 2002             TAPE 158
9      ISFN,FN1,FN2,IFNC,IFNG,IFNM,INDS,INEC,(DIK),K=2,6), TAPE 159
1      IPFGC,(LFGCCN(K),FGCL(K),K=1,IPFGC)           TAPE 160
C   TEST FOR PROPER DATA GROUP SERIAL NUMBER SEQUENCE ON TAPE          TAPE 161
C   TAPE 162
C   TAPE 163
C   IF (I = ISFN) 41,45,41             TAPE 164
41 REWIND 6                           TAPE 165
REWIND 8                           TAPE 166
C   TAPE 167
C   TAPE 168
C   TEST TO LIMIT THE NUMBER OF LINES PRINTED PER PAGE OF OUTPUT        TAPE 169
C   TAPE 170
C   IFIM = 52) 42,43,43               TAPE 171
43 WRITE OUTPUT TAPE 3, 3020          TAPE 172
C   ERROR PRINT - DATA GROUP SERIAL NUMBER INCONSISTENCY        TAPE 173
C   TAPE 174
-- 42 WRITE OUTPUT TAPE 3, 3005;          TAPE 175
9      ISFN,I             TAPE 176
GO TO 500                           TAPE 177
C   TAPE 178
C   BYPASS OF TESTS IF NO CARDS TO BE READ        TAPE 179
C   TAPE 180
C   45 IF (IPFM) 80,80,46             TAPE 181
C   TAPE 182
C   COMPUTATIONS FOR ADDITION OF INFORMATION TO TAPE 6          TAPE 183
C   TAPE 184
C   46 DO 47 L=1,IPFM               TAPE 185
C   TAPE 186
C   TEST FOR ALTERATIONS TO GROUP ISFN ON TAPE BY DATA FROM -G- CARD TAPE 187
C   TAPE 188
C   IF (I = LFNNIL) 47,50,47             TAPE 189
C   TAPE 190
47 CONTINUE                          TAPE 191
GO TO 80                           TAPE 192
C   TAPE 193
50 DO 51,J=L,200                    TAPE 194
C   TAPE 195
C   ZERO COUNT LIST STORAGE          TAPE 196
C   TAPE 197
51 FGCL(J) = 0.0                     TAPE 198
DO 52 K=1,IPFGC                   TAPE 199
C   TAPE 200
C   STORE TAPE VALUES OF THE NUMBER OF STRUCTURAL CONTRIBUTORS PER TAPE 201
.MOLECULE FOR EACH CONTRIBUTOR WITHIN THE SPECIFIED GROUP        TAPE 202
C   TAPE 203
J = LFGCCN(K)                      TAPE 204
52 FGCL(J) = FUCL(K)                TAPE 205
C   ADDITION OF NEW VALUES OF THE NUMBER OF STRUCTURAL CONTRIBUTIONS TAPE 206
.CONSEQUENTLY FOR THOSE CONTRIBUTORS LISTED ON THE -G- CARD        TAPE 207
C   TAPE 208
IPACC = LIPACC(J)                  TAPE 209
DO 53 K=1,IPACC                   TAPE 210
J = LACHN(L,K)                    TAPE 211
C   TAPE 212

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## SUBROUTINE TAPE

(CONTINUED)

## MASTER LIBRARY TAPE MODIFICATION

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53 FGCJL(J) = ACCL(L,K)
      K = 0
C   LIST CONTRIBUTOR CODE NUMBERS AND NUMBER OF CONTRIBUTORS PER
C... MOLECULE, TO BE WRITTEN ON TAPE.3
C
      DO 55 J=1,200
      IF (FGCJL(J)) 54,55,56
54 K = K+1
      LGCCN(K) = J
      FGCL(K) = FGCJL(J)
55 CONTINUE
      IPFGC = K
C   TEST TO LIMIT THE NUMBER OF LINES PRINTED PER PAGE OF OUTPUT
C
      IFIM + IPFGC/6 - 52, 53, 57, 57
57 WRITE OUTPUT TAPE 3, 3020
      M=0
58 M = M + IPFGC/6 + 6
C   PRINTOUT OF ALTERED LISTS
C
      WRITE OUTPUT TAPE 3, 3006
      WRITE OUTPUT TAPE 3, 3007
      9 ISFN, (LGCCN(K),FGCL(K),K=1,IPFGC)
C   INTERIM STORAGE ON TAPE 8
C
      80 WRITE OUTPUT TAPE 8, 2002
      9 ISFN,FN1,FN2,IFNC,IFNG,IFNM,INDS,INEC,(D(K),K=2,6)
      1 IPFGC,(LGCCN(K),FGCL(K),K=1,IPFGC)
90 CONTINUE
C   END OF ALTERATIONS AND ADDITIONS TO DATA GROUPS ON TAPE
C
C   ALTERATIONS OR ADDITIONS TO CONTRIBUTOR NAME LIST
C
C   READ CONTRIBUTOR NAMES AND DEPENDENT VARIABLE NAME LIST FROM TAPE
      READ INPUT TAPE 6, 2003
      9 (GNL(J),J=1,200)
      READ INPUT TAPE 6, 2003
      9 (DNM(K),K=1,6)
      REWIND 6
      REWIND 8
C   TEST FOR ALTERATION OR ADDITION
      IF (IPCN) 100,100,95
      9 H CARD HEADING
      95 READ INPUT TAPE 2, 1001,
          (JGNL(K),AGNL(K),K=1,IPCN)
C   TEST TO LIMIT THE NUMBER OF LINES PRINTED PER PAGE OF OUTPUT
C
      IFIM + IPCN/7 - 52, 97, 98, 98
      98 WRITE OUTPUT TAPE 3, 3020
      M=0
97 M=M + IPCN/7 + 6
C   PRINTOUT OF ALTERATIONS OR ADDITIONS TO CONTRIBUTOR NAME LIST
C
      WRITE OUTPUT TAPE 3, 3008
      WRITE OUTPUT TAPE 3, 3009
      9 (JGNL(K),AGNL(K),K=1,IPCN)
      DO 96 K=1,IPCN
      J = JGNL(K)
C   ADD ALTERED OR NEW NAMES TO LIST
      96 GNL(J) = AGNL(K)
C   REVISE GROUP COUNT
      100_IPI = IPI + IADD
C   PREPARE CORRECTED TAPE 6
      WRITE OUTPUT TAPE 6, 2000
      WRITE OUTPUT TAPE 6, 2001
      9 IPIN
C   (A) - CORRECTED GROUPS PREVIOUSLY ON TAPE
      9 DO 110 I = 1,IP1
      READ INPUT TAPE 8, 2002
      9 ISFN,FN1,FN2,IFNC,IFNG,IFNM,INDS,INEC,(D(K),K=2,6)
      1 IPFGC,(LGCCN(K),FGCL(K),K=1,IPFGC)
110 WRITE OUTPUT TAPE 6, 2002
      9 ISFN,FN1,FN2,IFNC,IFNG,IFNM,INDS,INEC,(D(K),K=2,6)
      1 IPFGC,(LGCCN(K),FGCL(K),K=1,IPFGC)
      1 IF ((IADD),115,115,117)
C   TEST TO LIMIT THE NUMBER OF LINES PRINTED PER PAGE OF OUTPUT
C
      115_IFIM - 56, 113, 119, 114
      114 WRITE OUTPUT TAPE 3, 3020
      M=0
      113 M=M+2
C   DIAGNOSTIC - NO NEW DATA GROUPS ADDED TO TAPE
C
      WRITE OUTPUT TAPE 3, 3011
      GO TO 140

```

## SUBROUTINE TAPE

(CONTINUED)

## MASTER LIBRARY TAPE MODIFICATION

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C   (B) - ADDITION OF NEW GROUPS TO TAPE          TAPE 319
C   TEST TO LIMIT THE NUMBER OF LINES PRINTED PER PAGE OF OUTPUT TAPE 320
C   117 IF(M = 52) L18,116,116                      TAPE 321
C   116 WRITE OUTPUT TAPE 3, 3020                   TAPE 322
C   M=0                                              TAPE 323
C   118 M=M+5                                         TAPE 324
C   PRINTOUT OF NEW GROUPS ADDED TO TAPE           TAPE 325
C   WRITE OUTPUT TAPE 3, 3012                         TAPE 326
C   120 DO 130 I=1,IADD                            TAPE 327
C       ISFN = IPI + 1                               TAPE 328
C       K1 = J4(I)
C       IF(M = 54) L29,128,128                      TAPE 329
C   128 WRITE OUTPUT TAPE 3, 3020                   TAPE 330
C   WRITE OUTPUT TAPE 3, 3012                         TAPE 331
C   M=0                                              TAPE 332
C   129 M=M+1                                         TAPE 333
C   WRITE OUTPUT TAPE 3, 3013                         TAPE 334
C       9     A1(I),A2(I),ISFN ,I1A(I),I1B(I),I1C(I),I2(I),I3(I),
C       1     DA(2,I),DA(3,I),DA(5,I),DA(6,I)          TAPE 335
C   130 WRITE OUTPUT TAPE 6, 2002                     TAPE 336
C       9     ISFN,A1(I),A2(I),I1A(I),I1B(I),I1C(I),I2(I),I3(I),
C       1     (DA(K,I),K=2,6),K1,(J1(K,I),B1(K,I),K=1,K1) TAPE 337
C   TEST TO LIMIT THE NUMBER OF LINES PRINTED PER PAGE OF OUTPUT TAPE 338
C   131 IF((M+14)/6 = 50) L31,132,132              TAPE 339
C   132 WRITE OUTPUT TAPE 3, 3020                   TAPE 340
C   M=0                                              TAPE 341
C   133 M=M+6                                         TAPE 342
C   WRITE OUTPUT TAPE 3, 3014                         TAPE 343
C   DO 135 I=1,IADD                                TAPE 344
C   ISFN = IPI + 1                               TAPE 345
C   K1 = J4(I)                                         TAPE 346
C   TEST TO LIMIT THE NUMBER OF LINES PRINTED PER PAGE OF OUTPUT TAPE 347
C   134 IF(M+14)/6 = 56) L33,134,134              TAPE 348
C   135 WRITE OUTPUT TAPE 3, 3020                   TAPE 349
C   WRITE OUTPUT TAPE 3, 3014                         TAPE 350
C   M=6                                              TAPE 351
C   136 M=M+14/I/6 + 2                            TAPE 352
C   135 WRITE OUTPUT TAPE 3, 3007                   TAPE 353
C       9     ISFN ,I1L(K,I),B1(K,I),K=1,K1)          TAPE 354
C   (C) - ADDITION OF CONTRIBUTOR NAME LIST TO TAPE TAPE 355
C   140 WRITE OUTPUT TAPE 6, 2003,                  TAPE 356
C       9     (GNL(I),J=1,200)                         TAPE 357
C   WRITE OUTPUT TAPE 6, 2003,                      TAPE 358
C       9     (DNN(K),K=1,6)                          TAPE 359
C   END FILE 6                                     TAPE 360
C   REWIND 6                                       TAPE 361
C   REWIND 8                                       TAPE 362
C   GO TO 500                                      TAPE 363
C   END OF OPERATIONS ON ALTERATIONS AND ADDITIONS TO TAPE 2 TAPE 364
C   OPERATIONS FOR INITIAL MAKEUP OF TAPE 2        TAPE 365
C   195 IF ((PCN),490,490,210                      TAPE 366
C   TITLE CARD READING                           TAPE 367
C   210 READ INPUT TAPE 2, 2000                   TAPE 368
C   M CARD READING                                TAPE 369
C   READ INPUT TAPE 2, 1001,                      TAPE 370
C       9     (JGNL(I),AGNL(K),K=1,|PCN|)            TAPE 371
C   DEPENDENT VARIABLE NAME LIST CARD READING    TAPE 372
C   READ INPUT TAPE 2, 1002,                      TAPE 373
C       9     (DNN(K),K=1,6),BLK                      TAPE 374
C   DO 215 J=1,200                                 TAPE 375
C   BLANK OUT ENTIRE CONTRIBUTOR NAME FIELD      TAPE 376
C   215 GNL(J) = BLK                               TAPE 377
C   DO 220 K=1,|PCN|                               TAPE 378
C   J = JGNL(K)                                     TAPE 379
C   STORE GROUPS FROM M CARD IN CONTRIBUTOR NAME FIELD TAPE 380
C   220 GNL(J) = AGNL(K)                          TAPE 381
C   IP ((IADD) 490,490,230                         TAPE 382
C   PRINTOUT OF INITIAL DATA FOR TAPE             TAPE 383
C   230 WRITE OUTPUT TAPE 3, 2000                  TAPE 384
C   WRITE OUTPUT TAPE 3, 3010,                      TAPE 385
C   WRITE OUTPUT TAPE 3, 3005,                      TAPE 386
C       9     (JGNL(I),AGNL(K),K=1;|PCN|)            TAPE 387
C   WRITE OUTPUT TAPE 3, 3015,                      TAPE 388
C       9     (DNN(K),K=1,6),BLK                      TAPE 389
C   PREPARE TAPE 6                                TAPE 390
C   WRITE OUTPUT TAPE 6, 2000,                      TAPE 391
C   WRITE OUTPUT TAPE 6, 2001,                      TAPE 392

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## SUBROUTINE TAPE

(CONTINUED)

## MASTER LIBRARY TAPE MODIFICATION

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9      IADD          TAPE 425
DO 240 I=1,IADD          TAPE 426
K1 = 14(1)          TAPE 427
240 WRITE OUTPUT TAPE 6, 2002,          TAPE 428
   9      1,(A1(I),A2(I),I1A(I),I1B(I),I1C(I),I2(I),I3(I)),          TAPE 429
   1,(DAIK(I),K2(6),K1,(J1K(I),BLK(I),K-1,K1))          TAPE 430
   WRITE OUTPUT TAPE 6, 2003,          TAPE 431
   9      (GNL(IJ),J=1,200)          TAPE 432
   WRITE OUTPUT TAPE 6, 2003,          TAPE 433
   (NNMK(I),K=1,6)          TAPE 434
END FILE 6          TAPE 435
WRITE OUTPUT TAPE 3, 3016          TAPE 436
REWIND 6          TAPE 437
C      END OF INITIAL PREPARATION OF TAPE 6          TAPE 438
C      GO TO 500          TAPE 439
C      ERROR PRINT - NO DATA FOR INITIAL TAPE PREPARATION          TAPE 440
C      TAPE 441
C      TAPE 442
C      TAPE 443
C      TAPE 444
490 WRITE OUTPUT TAPE 3, 3017,          TAPE 445
   9      IPCN,IADD          TAPE 446
495 REWIND 6,          TAPE 447
500 RETURN          TAPE 448
600 NEX = 2          TAPE 449
WRITE OUTPUT TAPE 3, 4000, IC, JII          TAPE 450
GO TO 500          TAPE 451
C      FORMAT STATEMENTS          TAPE 452
C      TAPE 453
C      TAPE 454
1001 FORMAT          TAPE 455
   9 (12X, ,I4,2X,A6,I4,2X,A6,I4,2X,A6,I4,2X,A6,I4,2X,A6)          TAPE 456
1002 FORMAT (12X, 7A6)          TAPE 457
2000 FORMAT (1H1,11X60H)          TAPE 458
1          TAPE 459
2001 FORMAT          TAPE 460
   9 (1H0,6(6))          TAPE 461
2002 FORMAT          TAPE 462
   9 (1H0,16,2A6,5T6,1P5E12.4,16/(1H 16,E12.4,16,E12.4,16,E12.4,16,
   1E12.4,16,E12.4,16,E12.4))          TAPE 463
2003 FORMAT          TAPE 464
   9 (1H0 9(6X,A6)/(1H 6X,A6,6X,A6,6X,A6,6X,A6,6X,A6,6X,A6,6X,A6,6X,
   1A6,6X,A6))          TAPE 465
3000 FORMAT          TAPE 466
   9 (1H1, ,3L1, 102MMONGANTO RESEARCH CORPORATION FLAME SPEED CALCULATI
   1ON - ROUTINE 2018 MODIFICATION 1 DATE 2A6 )          TAPE 467
3001 FORMAT          TAPE 471
   9 (1H0,10X, 38HTAPE 2 WRITING INFORMATION - RUN 14 )          TAPE 472
3002 FORMAT          TAPE 473
   9 (1H0,15X, 28H INITIAL TAPE PREPARATION )          TAPE 474
3003 FORMAT          TAPE 475
   9 (1H0, 16X,16X,30HDATA OUT OF ORDER - RUN NUMBER 14,
   1 14X,          20HMISPLACED RUN NUMBER 14,
   2 /1H0 16X,22HOPTION CONTROL INTEGER 14,
   3 22X,21HCONTROL INTEGER CHECK 14)          TAPE 476
3004 FORMAT          TAPE 477
   9 (1H0,10X, 20HNO ACTION CALLED FOR )          TAPE 478
3005 FORMAT          TAPE 479
   9 (1H0,10X, 57HGROUP SERIAL NUMBER INCONSISTENCY - SERIAL NUMB
   1ER = 14 + 5X, 11HLOCATION = 14.)          TAPE 480
3006 FORMAT          TAPE 481
   9 (1H0,10X, 34HALTERATIONS TO DATA GROUPS ON TAPE /
   1 1M 14M DATA GROUP /6X,11HCONTRIBUTOR,6X,11HCONTRIBUTOR,6X,11H
   2CONTRIBUTOR,6X,11HCONTRIBUTOR,6X,11HCONTRIBUTOR,6X,11HCONTRIBUTOR
   3/ 1M , 117H SERIAL CODE COUNT / CODE COUNT / CODE
   4 COUNT / CODE COUNT / CODE COUNT / CODE COUNT / CODE
   5/ 1M , 11H NUMBER MOLECULE NUMBER MOLECULE NUMBER MOLECULE NUMBER
   6R MOLECULE NUMBER MOLECULE NUMBER MOLECULE NUMBER MOLECULE /1)          TAPE 482
3007 FORMAT          TAPE 483
   9 (1H0, 110,7X, 6(16,2X,F7.3,2X)/(1H ,17X,16,2X,F7.3,2X,16,2X,F7.3
   1,2X,16,2X,F7.3,2X,16,2X,F7.3,2X,16,2X,F7.3,2X,16,2X,F7.3 )          TAPE 484
3008 FORMAT          TAPE 485
   9 (1H0,10X, 32HCHANGES IN CONTRIBUTOR NAME LIST )          TAPE 486
3009 FORMAT          TAPE 487
   9 (1H0,14H CONTRIBUTOR,6X,11HCONTRIBUTOR,6X,11H
   1CONTRIBUTOR,6X,11HCONTRIBUTOR,6X,11HCONTRIBUTOR,6X,11HCONTRIBUTOR
   2/ 1M + 5H CODE 13X,4HCODE 13X,4HCODE 13X,4HCODE 13X,4HCODE 13X,
   3 4HCODE 13X,4HCODE /          TAPE 488
   4 1M , 117NUMBER NAME NUMBER NAME NUMBER NAME NUMBER NAME NUMBER
   5R NAME NUMBER NAME NUMBER NAME NUMBER NAME NUMBER NAME NUMBER /
   6/ 1M , 16,2X,A6,3X,16,2X,A6,3X,16,2X,A6,3X,16,2X,A6,3X,16,2X,A6,3X
   7 16,2X,A6,3X,16,2X,A6,3X )          TAPE 489
3010 FORMAT          TAPE 490
   9 (1H0,10X, 29HINITIAL CONTRIBUTOR NAME LIST )          TAPE 491
3011 FORMAT          TAPE 492
   9 (1H0,10X, 32HNO NEW DATA GROUPS ADDED TO TAPE )          TAPE 493
3012 FORMAT          TAPE 494
   9 (1H0,10X, 25HDATA GROUPS ADDED TO TAPE /
   1 1M , 14H FUEL NAME 19X,12HCODE NUMBERS 22X,14HSTOICHIOMETRIC 11X
   2,13HMAXIMUM SPEED 4X,LINEQUivalence /1M ,13X,10HSERIAL CLASS G
   3ROUP MEMBER DATA EXPERIMENT FLAME FUEL FLAME
   4 FUEL RATIO AT /
   5 1M ,39X,77HSOURCE CONDITIONS SPEED CONCENTRATION SPEED
   6 CONCENTRATION - MAXIMUM /1M ,57X,6(1CM./SEC.) (MOLECULES/CC) .1CM.
   7/SEC) (MOLECULES/CC) FLAME SPEED /)          TAPE 495
3013 FORMAT          TAPE 496
   9 (1H , 2A6, 17,216,317, 4X, F9.4, 2X,1P12.4,2X,0PF9.4,2X,1P12.
   24,3X,1P12.4 )          TAPE 497
3014 FORMAT          TAPE 498
   9 (1H0,10X, 32HADDITIONS TO DATA GROUPS ON TAPE /
   1 1M ,14H DATA GROUP ,6X,11HCONTRIBUTOR,6X,11HCONTRIBUTOR,6X,11H
   2CONTRIBUTOR,6X,11HCONTRIBUTOR,6X,11HCONTRIBUTOR,6X,11HCONTRIBUTOR
   3/ 1M ,117H SERIAL CODE COUNT / CODE COUNT / CODE COUNT / CODE
   4 COUNT / CODE COUNT / CODE COUNT / CODE COUNT / CODE
   5/ 1M ,11H NUMBER MOLECULE NUMBER MOLECULE NUMBER MOLECULE NUMBER
   6R MOLECULE NUMBER MOLECULE NUMBER MOLECULE NUMBER MOLECULE /1)          TAPE 499

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SUBROUTINE CROUT
_____
MATRIX INVERSION FOR SUBROUTINE MAXM
_____
CCRT CROUT SUBROUTINE MOD 100 PROBLEM 2018 MARCH 1, 1962 MAR DAYTON CROUT 1
C CROUT 2
C Nomenclature CROUT 3
C CROUT 4
C DIVSH - NON-ZERO DIAGONAL ELEMENT DIVISION CROUT 5
C ID, JN, K, I, J - INDICES CROUT 6
C ITCTH - ITERATION COUNTER CROUT 7
C NVAR - NUMBER OF INDEPENDENT VARIABLES IN EQUATIONS CROUT 8
C W, WI(I), Y(I) - COEFFICIENTS (OUTPUT) CROUT 9
C Z, Z(I,J), X(I,J) - MATRIX OF INDEPENDENT VARIABLES (INPUT) CROUT 10
C CROUT 11
C CROUT 12
C SUBROUTINE CROUTINVAR(L,N)
DIMENSION X(10,111),Y(10),Z(10,111),W(10)
NVAR=1
1 DO 2 I=1,NVAR
DO 2 J=1,I,N
2 X(I,J)=Z(I,J)
ITCTH=0
3 I0= 1
C TEST FOR TWO OR MORE VARIABLES
C IF(NVAR-1)100,100,8
C TEST OF ZERO DIAGONAL ELEMENT
C 8 IF(X(ID, ID)) 9,11,9
9 DIVSH= X(ID, ID)
DO 10 J=ID,JN
10 X(I0,J)= X(ID,J)/DIVSH
11=ID+1
C INVERSION OF MATRIX
C DO 20 I=11,NVAR
DO 20 J=1,I,N
20 X(I,J)= X(I,J) - (X(ID,J)*(X(I, ID)))
IF (I0-JN+2)21,22,23
C SIGNAL FLAG TO INDICATE SOLUTION NOT POSSIBLE
C 23 SENSE LIGHT 4
GOTO 50
24 ID=ID+1
GO TO 10
22 I0= ID +1
C TEST FOR ZERO DIAGONAL ELEMENT
C IF(X(ID, ID)) 24,11,24
C SIGNAL FLAG TO INDICATE SOLUTION NOT POSSIBLE
C 11 SENSE LIGHT 3
GO TO 50
24 DIVSH = X(ID, ID)
C INVERSION OF MATRIX
C DO 25 J= ID,JN
25 X(ID,J)= X(I0,J)/DIVSH
K=NVAR
Y(K)= X(NVAR, JN)
126 IF(K-1)150,150,26
26 K =K-1
Y(K) = X(K, JN)
J1= K+1
DO 30 J=J1,NVAR
30 Y(K) = Y(K) - (X(K,J))*(Y(J))
GO TO 126
50 RETURN
100 WI(I)= X(I, 1)/X(1, 1)
IF DIVIDE CHECK 11, 50
150 IF (ITCTH) 151,151,200
C COEFFICIENT STORAGE IN OUTPUT VECTOR
C 151 DO 352 I=1,NVAR
352 W (I) = Y(I)
GO TO 251
200 DO 201 I=1,NVAR
201 WI(I)= W(I) - Y(I)
C TEST FOR SATISFACTORY COMPLETION OF SOLUTION
C IF(ITCTH-3)251,90,50
251 ITCTH = ITCTH +1
DO 152 I = 1,NVAR
DO 152 J = 1,NVAR
152 X(I,J) = Z(I,J)
DO 153 I = 1,NVAR
X (I,JN) = -1.0 * Z (I,JN)
DO 153 J = 1,NVAR
153 X(I,JN) = X(I,JN) - (X(I,J)*(WI(J)))
GO TO 3
END

```

## SUBROUTINE FSCI

## DATA CARD INPUT

CFSCI	DATA CARD INPUT SUBROUTINE FOR FLAME SPEED CALCULATIONS	FSCI	1
	SUBROUTINE INPUT	FSCI	2
	COMMON INT, DEC, IC, J11, J2, J3, NIN, NEX	FSCI	3
	DIMENSION INT(10), DEC(10), KARRAY(10), PARRAY(10)	FSCI	4
	NIN = NIN	FSCI	5
4	NUMDCP = 3	FSCI	6
	KPASS = 0	FSCI	7
401	KPASS = KPASS+1	FSCI	8
	CALL VDECOM(NUMDCP, KARRAY, PARRAY, KPASS)	FSCI	9
	GU 10 402, 405, 410, KPASS	FSCI	10
402	I = KARRAY(1)	FSCI	11
	IC = 1	FSCI	12
	L = 1/1000	FSCI	13
	IF( IC) 4020, 4, 4020	FSCI	14
4020	J11 = KARRAY(2)	FSCI	15
	J2= KARRAY(3)	FSCI	16
	NUMDCP = J2 + 1	FSCI	17
	GO TO 401	FSCI	18
405	UU 406, J=1..J2	FSCI	19
406	IINT(J) = KARRAY(J)	FSCI	20
	J3 = *KARRAY(J2+1)	FSCI	21
	NUMDCP = J3	FSCI	22
	GG TO 401	FSCI	23
410	UU 412, J=1..J3	FSCI	24
412	DEC(J) = PARRAY(J)	FSCI	25
	NEX = L	FSCI	26
	GU TO 1 50, 60), NIN	FSCI	27
49	NIN = 1	FSCI	28
50	RETURN	FSCI	29
60	IF( IC = 1000) 4, 49, 4	FSCI	30
	END	FSCI	31

## SUBROUTINE VDECOM

## INTEGER INPUT DATA DECOMPOSITION

```

SUBROUTINE VDECOM(IN, KARRAY, P, KPASS) VDECOM 1
DIMENSION P(101) VDECOM 2
DIMENSION DUMMY(30), DUMMY1(30) VDECOM 3
DIMENSION KINPUT(72), KARRAY(101), PARRAY(101), AINPUT(72). VDECOM 4
1 KOUTPT(72), AOUTPT(72) VDECOM 5
COMMON IJUNNY, IPLUS, IMINUS, IDECPT, ICOMMA, IE, IBLANK, VDECOM 6
1 KINPUT, NUNDSP, PARRAY, I, L, NEX, NI VDECOM 7
EQUIVALENCE I DUMMY, IJUNNY I VDECOM 8
1 ,IPLUS,IPLUS,(AMINUS,IMINUS), (DECPT,IDECP), VDECOM 9
1 (COMMA,ICOMMA),(IE,IBLANK,ILANBLK,ILANML) VDECOM 10
2 (AINPUT, KINPUT), (AOUTPT, KOUTPT) VDECOM 11
REWIND 5 VDECOM 12
NUNDSP = N VDECOM 13
NEX = 1 VDECOM 14
NI = 1 VDECOM 15
I = 1 VDECOM 16
GO TO( 1,10, 50), KPASS VDECOM 17
1 CONTINUE VDECOM 18
C SET UP CHARACTERS FOR LATER TEST VDECOM 19
B PLUS = 2060000000000 VDECOM 20
B AMINUS = 4060000000000 VDECOM 21
B DECPT = 3260000000000 VDECOM 22
B COMMA = 7360000000000 VDECOM 23
B E = 2560000000000 VDECOM 24
B BLANK = 6060000000000 VDECOM 25
C READ ALPHANUMERIC CHARACTERS VDECOM 26
5 READ INPUT TAPE 2,1000, (AINPUT(J),J=1,72) VDECOM 27
1a GO TO(10, 10, 50), KPASS VDECOM 28
C DECOMPOSITION OF INTEGERS VDECOM 29
10 DO 21 N = NI, NUNDSP VDECOM 30
21 NI = N VDECOM 31
C SEARCH FOR START OF NUMBER VDECOM 32
101 IF (KINPUT(I) = IBLANK) 102, 11, 102 VDECOM 33
102 IF (KINPUT(I) = ICOMMA) 12, 11, 12 VDECOM 34
11 I = I+1 VDECOM 35
IFI = -72)101,101, 5 VDECOM 36
C SELECT INTEGERS VDECOM 37
12 LI = 1 VDECOM 38
M = 0 VDECOM 39
DO 20 J=1,6 VDECOM 40
KOUTPT(LI) = KINPUT(I) VDECOM 41
IFI(KINPUT(I) = IBLANK)121..13..121 VDECOM 42
IFI(KINPUT(I) = ICOMMA) 122, 120, 122 VDECOM 43
122 IFI KINPUT(I) = IPLUS) 123, 120, 123 VDECOM 44
120 M = 1 VDECOM 45
123 I = I+1 VDECOM 46
I = I+1 VDECOM 47
IFI(KINPUT(I) = IBLANK)121..13..121 VDECOM 48
171 IFI(KINPUT(I) = ICOMMA) 20, 13 ..20 VDECOM 49
C RIGHT ADJUST IN FIELD VDECOM 50
13 IFI J=6) 14,21,14 VDECOM 51
14 KDO = J - M VDECOM 52
DO 15 K = 1, KDO VDECOM 53
L2 = LI + 6 - K VDECOM 54
15 I = I+1 - K VDECOM 55
15 KOUTPT( L2 ) = KOUTPT( L3 ) VDECOM 56
L = LI + A VDECOM 57
KDO = 6-J + M VDECOM 58
KDO = 1 + M VDECOM 59
DO 16 K = KDO, KDO VDECOM 60
14 = LI + K - 1 VDECOM 61
16 KOUTPT( L4 ) = 0 VDECOM 62
GO TO 21 VDECOM 63
20 CONTINUE VDECOM 64
21 CONTINUE VDECOM 65
IEND = 6+ NUNDSP VDECOM 66
C WRITE ALPHANUMERIC CHARACTERS VDECOM 67
WRITE OUTPUT TAPE 5,1000, (AOUTPT(J), J=1, IEND) VDECOM 68
REWIND 5 VDECOM 69
C READ INTEGER LIST VDECOM 70
READ INPUT TAPE 5,1001, (KARRAY(I), I=1,NUNDSP) VDECOM 71
REWIND 5 VDECOM 72
40 RETURN VDECOM 73
50 CALL DECOP VDECOM 74
NEX = NEX VDECOM 75
GO TO(30,5), NEX VDECOM 76
30 DO 31 J = 1, NUNDSP VDECOM 77
31 P(IJ) = PARRAY(IJ) VDECOM 78
GO TO 40 VDECOM 79
1000 FORMAT(72A1) VDECOM 80
1001 FORMAT(11I6) VDECOM 81
END VDECOM 82

```

## SUBROUTINE DECOCP

## FLOATING POINT INPUT DATA DECOMPOSITION

```

SUBROUTINE DECOCP
COMMON IDUMMY, IPLUS, I_MINUS, IDECP, ICNMA, IE, ISBLANK,
1 KINPUT, NUMDCP, PARRAY, I, L, NEX, NI
EQUIVALENCE (DUMMY, IDUMMY)
EQUIVALENCE (AOUTPT, KOUTPT)
DIMENSION AOUTPT(172), KOUTPT(172), PARRAY(101), KINPUT(172)
DIMENSION IDUMMY(30), DUMMY(30)
NEX = NEX
M = L
GO TO 150,511,NEX
C DECOMPOSITION OF DECIMAL AND EXPONENTIAL NUMBERS
C LIMIT DECOMPOSITION ID & NUMBERS
50 IF(INUHDCP = 6)503,503,502
502 IDEC = 6
IEND = 12+IDECP
GO TO 504
503 IDEC = NUMDCP
IEND = 12+NUMDCP
504 IF(I = 72)51,51,505
505 NEX = 2
GO TO 300
51 NEX = 1
DO 100 NI = NI, IDEC
NI = N
C SEARCH FOR START OF NUMBER
510 IF(KINPUT(I) = ISBLANK)52,53,52
52 IF(KINPUT(I) = ICNMA)54,53,54
53 I = I + 1
IF(I = 72)510,510,505
54 NI = M
C STORE NUMBERS UP TO DECIMAL POINT
541 IF(KINPUT(I)) = IDECP)55,65,55
55 KOUTPT(M) = KINPUT(I)
I = I + 1
M = M + 1
GO TO 541
C TEST FOR END OF NUMBER OR EXPONENTIAL
60 IF(KINPUT(I)) = IE)61,70,61
61 IF(KINPUT(I)) = IPLUS)62,70,62
62 IF(KINPUT(I)) = I_MINUS)63,70,63
63 IF(KINPUT(I)) = ICNMA)64,80,64
64 IF(KINPUT(I)) = ISBLANK)65,80,65
C STORE DECIMAL POINT AND NUMBERS
65 KOUTPT(M) = KINPUT(I)
I = I + 1
M = M + 1
GO TO 60
C COMPLETE EXPONENTIAL FIELD..THROUGH R LOCATIONS
70 LDO = M1 + 7
DO 71 J1 = M, LDO
71 KOUTPT(J1) = 0
M = M1 + 8
C STORE E IN LOCATION 9
KOUTPT(M) = IE
IE(KINPUT(I)) = IE)73,72,73
72 I = I + 1
C TEST FOR SIGN OF EXPONENT
73 IF(KINPUT(I)) = I_MINUS)74,76,74
74 IF(KINPUT(I)) = IPLUS)75,76,75
75 KOUTPT(M+1) = IPLUS
GO TO 77
C STORE SIGN
76 KOUTPT(M+1) = KINPUT(I)
I = I + 1
C TEST FOR END OF EXPONENT
77 IF(KINPUT(I+1) = ISBLANK)78,79,78
78 IF(KINPUT(I+1) = ICNMA)79,79,79
79 KOUTPT(M+2) = 0
KOUTPT(M+3) = KINPUT(I)
GO TO 792
791 KOUTPT(M+2) = KINPUT(I)
KOUTPT(M+3) = KINPUT(I+1)
792 I = I + 2
M = M1 + 12
GO TO 100
C COMPLETE DECIMAL FIELD
80 LDO = M1 + 11
DO 81 J1 = M, LDO
81 KOUTPT(J1) = 0
M = M1 + 12
100 CONTINUE
C WRITE ALPHANUMERIC CHARACTERS
WRITE OUTPUT TAPE 5,1000,(AOUTPT(J1),J=1,IEND)
IF(INUHDCP = IDEC)201,201,200
200 NEX = 1
NI = NI + 1
IEND = 12+INUHDCP - 6
IDECP = NUMDCP
GO TO 504
201 REWIND 5
C READ DECIMAL AND EXPONENTIAL LIST
READ INPUT TAPE 5,1010,(PARRAY(J),J=1,NUHDCP)
REWIND 5
300 L = M
RETURN
1000 FORMAT(172A11)
1010 FORMAT(16F12.5)
END

```

PCASANTO RESEARCH CORPORATION FLAME SPEED CALCULATOR - ROUTINE 2010 MODIFICATION 1 RUN 735 DATE 5/5/61

INPUT DATA

FUEL NAME	INHIBITORS USED
HYDROGEN	
FUEL CLASS NUMBER	FUEL GROUP NUMBER
C	0
DATA SOURCE NUMBER	EXPERIMENTAL CONDITIONS NUMBER
1	1
FLAME VELOCITY AT STOICHIOMETRIC CONCENTRATION RATIO	CM./SEC.
0.	0.
MAXIMUM FLAME VELOCITY	CM./SEC.
0.	0.
FUEL CONCENTRATION AT STOICHIOMETRIC CONDITIONS	MOLECULES/CC.
0.	0.
FUEL CONCENTRATION AT CONDITIONS OF MAXIMUM VELOCITY	MOLECULES/CC.
0.	0.
EQUIVALENCE RATIO AT MAXIMUM FLAME SPEED	0.
SPECIES CONTRIBUTOR CODE NUMBER	NUMBER OF CONTRIBUTORS PER MOLECULE OF FUEL
1	2.000
2	2.000
3	3.000
4	2.000
5	4.000
6	5.000
7	6.000
	7.000

## EXPERIMENTAL DATA

MIXTURE TEMPERATURE 25.0 DEG. C. MIXTURE PRESSURE 760.0 MM. MERCURY

ATOMS OF OXYGEN TO COMPLETELY OXIDIZE ONE MOLE OF FUEL 1.00

MOLE FRACTION OXYGEN IN OXIDANT 0.2100

VOLUME PER MOLE OF FUEL 2.2414E 04 CC. PER GRAM-HOLE

## FLAME FRONT DIMENSIONS

RUN

738 PEAK HEIGHT (MEASURED UNITS) 69.00

STATION (MEASURED)	1	2	3	4	5
DIAMETER (MEASURED)	41.000	30.000	21.000	14.000	6.500
HEIGHT (CM.)	0.	0.20000	0.40000	0.60000	0.80000
DIAMETER (CM.)	0.61538	0.45280	0.31520	0.21013	0.09750
ACTUAL LENGTH OF REFERENCE	4.00000	CM.		MEASURED LENGTH OF REFERENCE	266.50000 UNITS

738 PEAK HEIGHT (MEASURED UNITS) 62.00

STATION (MEASURED)	1	2	3	4	5
DIAMETER (MEASURED)	40.500	30.000	21.000	13.500	6.500
HEIGHT (CM.)	0.	0.20000	0.40000	0.60000	0.80000
DIAMETER (CM.)	0.60780	0.45280	0.31520	0.20263	0.09750
ACTUAL LENGTH OF REFERENCE	4.00000	CM.		MEASURED LENGTH OF REFERENCE	266.50000 UNITS

737 PEAK HEIGHT (MEASURED UNITS) 65.00

STATION (MEASURED)	1	2	3	4	5
DIAMETER (MEASURED)	42.000	31.000	22.000	15.000	8.000
HEIGHT (CM.)	0.	0.20000	0.40000	0.60000	0.80000
DIAMETER (CM.)	0.63516	0.46681	0.33270	0.22684	0.12098
ACTUAL LENGTH OF REFERENCE	4.00000	CM.		MEASURED LENGTH OF REFERENCE	264.50000 UNITS

736 PEAK HEIGHT (MEASURED UNITS) 73.00

STATION (MEASURED)	1	2	3	4	5	6
DIAMETER (MEASURED)	42.000	32.500	25.000	18.000	11.500	5.500
HEIGHT (CM.)	0.	0.20000	0.40000	0.60000	0.80000	1.00000
DIAMETER (CM.)	0.63277	0.48544	0.36158	0.27115	0.17324	0.08280
ACTUAL LENGTH OF REFERENCE	4.00000	CM.		MEASURED LENGTH OF REFERENCE	265.50000 UNITS	

739 PEAK HEIGHT (MEASURED UNITS) 79.00

STATION (MEASURED)	1	2	3	4	5	6
DIAMETER (MEASURED)	41.500	32.500	25.000	18.500	11.500	5.500
HEIGHT (CM.)	0.	0.20000	0.40000	0.60000	0.80000	1.00000
DIAMETER (CM.)	0.62524	0.48564	0.37665	0.27872	0.17326	0.08286
ACTUAL LENGTH OF REFERENCE	4.00000	CM.		MEASURED LENGTH OF REFERENCE	265.50000 UNITS	

740 PEAK HEIGHT (MEASURED UNITS) 75.00

STATION (MEASURED)	1	2	3	4	5	6
DIAMETER (MEASURED)	42.500	34.000	26.000	19.000	12.500	7.000
HEIGHT (CM.)	0.	0.20000	0.40000	0.60000	0.80000	1.00000
DIAMETER (CM.)	0.63315	0.50652	0.38734	0.28305	0.18622	0.10428
ACTUAL LENGTH OF REFERENCE	4.00000	CM.		MEASURED LENGTH OF REFERENCE	268.50000 UNITS	

741 PEAK HEIGHT (MEASURED UNITS) 77.00

STATION (MEASURED)	1	2	3	4	5	6
DIAMETER (MEASURED)	43.000	36.000	27.000	21.000	15.000	8.500
HEIGHT (CM.)	0.	0.20000	0.40000	0.60000	0.80000	1.00000
DIAMETER (CM.)	0.64259	0.53832	0.40374	0.31402	0.22430	0.12710
ACTUAL LENGTH OF REFERENCE	4.00000	CM.		MEASURED LENGTH OF REFERENCE	267.50000 UNITS	

742 PEAK HEIGHT (MEASURED UNITS) 88.00

STATION (MEASURED)	1	2	3	4	5	6	7
DIAMETER (MEASURED)	44.000	37.000	30.500	24.000	17.500	13.000	7.000
HEIGHT (CM.)	0.	0.20000	0.40000	0.60000	0.80000	1.00000	1.20000
DIAMETER (CM.)	0.65549	0.55121	0.45438	0.35754	0.26071	0.19367	0.10428
ACTUAL LENGTH OF REFERENCE	4.00000	CM.		MEASURED LENGTH OF REFERENCE	266.50000 UNITS		

RUN	FUEL FLOW (CC./SEC.)	OXIDANT FLOW (CC./SEC.)	MOLE FRACTION INHIBITOR (CC./SEC.)	VOLUME FLOW (CC./SEC.)	CCNE AREA (SQ. CM.)	FLAME SPEED (CM./SEC.)	EQUIVALENCE RATIO
735	75.20000	137.30000	0.	231.95763	0.91660	254.73346	1.30404
736	91.40000	137.30000	0.	249.64099	0.89899	277.68917	1.58499
737	107.60000	137.30000	0.	267.32435	0.92310	274.71471	1.06592
738	124.00000	137.30000	0.	285.22602	1.09941	259.43550	2.15031
739	124.00000	126.80000	0.	273.76458	1.16800	247.07953	2.32038
740	124.00000	116.50000	0.	262.92146	1.15208	227.86642	2.93423
741	124.00000	106.20000	0.	251.27834	1.24648	201.85869	2.78002
742	124.00000	86.00000	0.	229.22872	1.43982	159.26607	3.43300

## FLAME SPEED CURVE DATA

A1 -3.8707E C2	A2 7.9649E C2	A3 -3.2718E 02	A4 4.1656E 01	STANDARD DEVIATION. A1 MAX. FLAME SPEED 1.5729	EQUIVALENCE RATIO A1 MAX. FLAME SPEED 1.7228	MAXIMUM FLAME SPEED 278.0486	COEFFICIENTS	
							A5	A6
735	1.3641	294.7315	295.3638	-0.6324	-0.2476			
736	1.5820	271.6802	275.8121	1.6771	0.6604			
737	1.8659	274.7147	275.8816	-1.1669	-0.4230			
738	2.1561	259.6355	260.4419	-1.5265	-0.3468			
739	2.3284	247.0795	246.2792	0.8063	0.3290			
740	2.5242	222.8664	224.4501	1.2163	0.3364			
741	2.7066	201.9587	202.2344	-0.6717	-0.3361			
742	3.0230	152.2061	152.1984	0.0077	0.0268			

DATA ACCEPTABLE		INHIBITORS USED	
FUEL NAME			
<u>HYDROGEN</u>			
FUEL CLASS NUMBER	C	FUEL GROUP NUMBER	D
CATA_SOURCE_NUMBER	1	EXPERIMENTAL CONCITIONS NUMBER	1
FLAME VELOCITY AT STOICHIOMETRIC CONCENTRATION RATIO	203.8527	CM./SEC.	
MAXIMUM FLAME VELOCITY	278.0484	CM./SEC	
FUEL CONCENTRATION AT STOICHIOMETRIC CONDITIONS	0.728220E.19	MOLECULES/CC.	
FUEL CONCENTRATION AT CONDITIONS OF MAXIMUM VELOCITY	0.103363E 20	MOLECULES/CC.	
EQUIVALENCE RATIO AT MAXIMUM FLAME SPEED	1.72208		

APPENDIX B

Fortran program and Sample Printouts  
for Routine FSR

ROUTINE FSR			
FLAME SPEED REGRESSION CALCULATIONS			
* 062-215	10000	7 O.S. MAC7617 RINGROSE	
*	LISTS	FSR 1	
*	SYMBOL TABLE	FSR 2	
CFSR	FLAME SPEED REGRESSION ROUTINE 1922A MAC - DAYTON MARCH 12, 1962	FSR 3	
C	NOMENCLATURE	FSR 4	
C	CGC(K,KUV)	- INPUT LIST OF PRESPECIFIED CONTRIBUTOR COEFFICIENTS	FSR 5
C	CGC(J,J)	- LIST OF PRESPECIFIED COEFFICIENTS	FSR 6
C	DIX(J)	- FLAME SPEED DATA	FSR 7
C	DNMK(K)	- NAME LIST OF DEPENDENT VARIABLE COMPONENTS	FSR 8
C	FCCJ(J)	- INTERNAL FULL LIST OF CONTRIBUTOR COUNTS	FSR 9
C	FCCL(K)	- INPUT TAPE LIST OF CONTRIBUTOR COUNTS	FSR 10
C	FN1 AND FN2	- FIRST AND SECOND HALVES OF FUEL NAME (ON TAPE)	FSR 11
C	FN1LN(J) AND	- FIRST AND SECOND HALVES OF ACCEPTED FUEL NAMES LIST	FSR 12
C	FN2LN(J)	- FIRST AND SECOND HALVES OF ACCEPTED FUEL NAMES LIST	FSR 13
C	GNL(J)	- INPUT TAPE LIST OF CONTRIBUTOR NAMES	FSR 14
C	I	- DATA SERIAL NUMBER INDEX	FSR 15
C	ICFN	- FUEL CLASS NUMBER (ON TAPE)	FSR 16
C	IGFN	- FUEL GROUP NUMBER (ON TAPE)	FSR 17
C	IMFN	- FUEL MEMBER NUMBER (ON TAPE)	FSR 18
C	INDS	- DATA SOURCE NUMBER (ON TAPE)	FSR 19
C	INEC	- EXPERIMENTAL CONDITIONS NUMBER (ON TAPE)	FSR 20
C	IPCFN	- NUMBER OF ENTRIES IN INPUT LIST OF ACCEPTABLE FUEL CLASS NUMBERS	FSR 21
C	IPCTC	- NUMBER OF ENTRIES IN INPUT LIST OF CONDITIONAL TEST CRITERIA	FSR 22
C	IPCTC9	- NUMBER OF CONDITIONAL TESTS + 3	FSR 23
C	IPDV	- NUMBER OF DEPENDENT VARIABLES TO BE REGRESSED	FSR 24
C	IPCGC	- NUMBER OF ENTRIES IN (KDVT) LIST OF PRESPECIFIED COEFFICIENTS	FSR 25
C	IPGFN	- NUMBER OF ENTRIES IN INPUT LIST OF ACCEPTABLE FUEL CLASS-GROUP NUMBERS	FSR 26
C	IP1	- NUMBER OF DATA GROUPS ON TAPE 2	FSR 27
C	IPIGTN	- NUMBER OF DUAL ENTRIES IN INPUT LIST OF CONTRIBUTION TESTS	FSR 28
C	IPJ	- HIGHEST VALUE OF CONTRIBUTOR NUMBER INDEX	FSR 29
C	IPLAG	- NUMBER OF DUAL ENTRIES IN INPUT LIST OF INTEGERS TO OVERRIDE REGRESSION CONTROL DATA	FSR 30
C	IPN	- NUMBER OF INDEPENDENT VARIABLES FOR REGRESSION	FSR 31
C	IPMC	- NUMBER OF PRESPECIFIED COEFFICIENTS IN REGRESSION DATA	FSR 32
C	IPMPN	- NUMBER OF ENTRIES IN INPUT LIST OF UNACCEPTABLE FUEL MEMBER NUMBERS	FSR 33
C	IPN	- NUMBER OF ACCEPTED DATA GROUPS FOR REGRESSION	FSR 34
C	IPRCL	- NUMBER OF ENTRIES IN INPUT LIST OF DECIMAL DATA TO OVERRIDE REGRESSION CONTROL DATA	FSR 35
C	IPSFN	- NUMBER OF ENTRIES IN INPUT LIST OF ACCEPTABLE DATA SERIAL NUMBERS	FSR 36
C	ISPN	- DATA GROUP SERIAL NUMBER (ON TAPE)	FSR 37
C	J	- CONTRIBUTOR NUMBER INDEX	FSR 38
C	J1, J2, K, L,	- INDICES	FSR 39
C	M1 AND N2	- CONTRIBUTOR COUNT TEST NUMBER	FSR 40
C	JGTM	- CONTRIBUTOR STATUS	FSR 41
C	JIN(J)	- (1 = POSSIBLE, 0 = OMIT, 1 = INCLUDE; 2 = INCLUDE COEFFICIENT PRESPECIFIED)	FSR 42
C	KDV	- DEPENDENT VARIABLE INDEX (PROBLEM NUMBER)	FSR 43
C	KDVO	- DEPENDENT VARIABLE DENOMINATOR IDENTIFICATION NUMBER	FSR 44
C	KOVN	- DEPENDENT VARIABLE NUMERATOR IDENTIFICATION NUMBER	FSR 45
C	KSFE	- DEPENDENT VARIABLE SCALE FACTOR EXPONENT	FSR 46
C	LCGN(MC)	- LIST OF ACCEPTED CONTRIBUTOR NUMBERS HAVING PRESPECIFIED COEFFICIENTS	FSR 47
C	LCFN(K)	- INPUT LIST OF ACCEPTABLE FUEL CLASS NUMBERS	FSR 48
C	LCGCN(K,KDV)	- INPUT LIST OF CONTRIBUTOR CODE NUMBERS HAVING PRESPECIFIED COEFFICIENTS	FSR 49
C	LCFC(K)	- INPUT LIST OF CONDITIONAL TEST CRITERIA	FSR 50
C	LDV(DKDV)	- INPUT LIST OF DEPENDENT VARIABLE DENOMINATOR NUMBERS	FSR 51
C	LDVN(KDV)	- INPUT LIST OF DEPENDENT VARIABLE NUMERATOR NUMBERS	FSR 52
C	LFGCCN(K)	- INPUT TAPE LIST OF CONTRIBUTOR CODE NUMBERS HAVING POSITIVE COUNTS	FSR 53
C	LGFN(L,K)	- INPUT LIST OF ACCEPTABLE FUEL CLASS-GROUP NUMBERS	FSR 54
C	LGTN(J)	- FULL LIST OF CONTRIBUTOR COUNT TEST NUMBERS 10 - OMIT, 1 - ACCEPT, 2 - REJECT GROUP IF COUNT NOT ZERO, 3 - REJECT GROUP IF ZERO, 4 TO 9 - CONDITIONAL TESTS	FSR 55
C	LIGTCN(K)	- INPUT LIST OF CONTRIBUTOR NUMBERS HAVING COUNT TEST ENTRIES	FSR 56
C	LIGTN(K)	- INPUT LIST OF CONTRIBUTOR COUNT TEST NUMBERS	FSR 57
C	LIPCGC(KDV)	- INPUT LIST OF NUMBER OF ENTRY PAIRS OF PRESPECIFIED REGRESSION COEFFICIENTS	FSR 58
C	LIVCN(M)	- LIST OF ACCEPTED INDEPENDENT CONTRIBUTOR NUMBERS	FSR 59
C	LNPHN(K)	- INPUT LIST OF UNACCEPTABLE FUEL CLASS-GROUP MEMBER NUMBERS	FSR 60
C	LOKSPN(M)	- LIST OF ACCEPTED DATA SERIAL NUMBERS	FSR 61
C	LRCK(K)	- INPUT LIST OF OVERRIDING INTEGER REGRESSION CONTROL DATA	FSR 62
C	LCGCK(K)	- LIST OF INTEGER REGRESSION CONTROL DATA	FSR 63
C	LSPN(K)	- INPUT LIST OF ACCEPTABLE DATA NUMBERS	FSR 64
C	M	- INDEX OF ACCEPTED CONTRIBUTORS WITHOUT PRESPECIFIED COEFFICIENTS	FSR 65
C	NC	- INDEX OF ACCEPTED CONTRIBUTORS WITH PRESPECIFIED COEFFICIENTS	FSR 66
C	N	- INDEX OF ACCEPTED DATA GROUPS	FSR 67
C	NOS	- ACCEPTABLE DATA SOURCE NUMBER	FSR 68

ROUTINE	FSR	(CONTINUED)
FLAME SPEED REGRESSION CALCULATIONS		
C	I_0 - ALL SOURCES ACCEPTABLE	FSR 105
C	1,2,ETC - ONLY SOURCES ACCEPTABLE)	FSR 106
C	NEC - ACCEPTABLE EXPERIMENTAL CONDITIONS NUMBER	FSR 107
C	(0 - ALL SOURCES ACCEPTABLE	FSR 108
C	1,2,ETC - ONLY SOURCES ACCEPTABLE)	FSR 109
C	NOL(K) - COLUMN HEADINGS FOR INDEPENDENT CONTRIBUTORS	FSR 110
C	TABLE	FSR 111
C	NRCI(K) - INPUT LIST OF OVERRIDING INTEGER REGRESSION	FSR 112
C	DATA INDICES	FSR 113
C	NSER - RUN NUMBER	FSR 114
C	NNZ(K) - CUMULATIVE SUM OF NON-ZERO VALUES OF	FSR 115
C	CONTRIBUTOR COUNT INDEX (K)	FSR 116
C	NZ(K) - CUMULATIVE SUM OF ZERO VALUES OF CONTRIBUTOR	FSR 117
C	COUNT INDEX (K)	FSR 118
C	OCDNL(MC) - ACCEPTABLE INDEPENDENT CONTRIBUTOR NAMES	FSR 119
C	OGNL(N) - NAMES OF ACCEPTED CONTRIBUTORS WITH	FSR 120
C	PRESPECIFIED COEFFICIENTS	FSR 121
C	OPL(I) - LIST OF INDEPENDENT CONTRIBUTOR COUNTS	FSR 122
C	PFAIL - REGRESSION VALIDITY INDICATOR	FSR 123
C	(0,0 - ACCEPTABLE, 1,0 - UNACCEPTABLE )	FSR 124
C	RCGL(K) - LIST OF DECIMAL REGRESSION CONTROL DATA	FSR 125
C	V - DEPENDENT VARIABLE (BEFORE OR AFTER	FSR 126
C	COEFFICIENT ADJUSTMENT)	FSR 127
C	YMAX(K) - MAXIMUM ABSOLUTE VALUE OF Y ENCOUNTERED	FSR 128
C		FSR 129
COMMON INT, DEC, IC, J1, J2, J3, NIN, NEX		FSR 130
DIMENSION INIT(10), DECL(10)		FSR 131
DIMENSION CGC(50,10), CGCJ(200), D(6), DN(6), FGCJ(200),		FSR 132
1 FGCL(90), FNLL(300), GNL(200), OCDNL(50),		FSR 133
2 UGNL(100), OPL(57), RCCL(3), YM(10),		FSR 134
3 JIN(200), LCCN(150), LCFN(20), LGCCN(50,10), LTC(9),		FSR 135
4 LDV(10), LDVN(10), LFGCN(140), LGFN(2,40), LGTN(200),		FSR 136
5 LGTCN(50), LGTN(50), LPFCN(10), LMFN(100), LMFN(100),		FSR 137
6 LOKSN(300), LRCT(11), LSPN(300), NN(19), NOL(10),		FSR 138
7 NRCI(11), NZ(9), COEN(100)		FSR 139
C	SETUP OF COLUMN HEADINGS FOR INDEPENDENT CONTRIBUTORS TABLE	FSR 140
C		FSR 141
DO 14 K=1,10		FSR 142
19 NOL(K) = K-1		FSR 143
PFAIL = 0.0		FSR 144
REWIND 7		FSR 145
REWIND 8		FSR 146
REWIND 6		FSR 147
C	SETUP FOR SCALE FACTOR CALCULATIONS	FSR 148
C		FSR 149
20 DO 21 K=1,10		FSR 150
21 YM(K) = 0.0		FSR 151
C	SETUP OF CONTRIBUTOR STATUS LIST TO -POSSIBLE- CONDITION	FSR 152
C	-1 POSSIBLE, 0 OMIT, 1 INCLUDE,	FSR 153
C	2 INCLUDE (COEFFICIENT PRESPECIFIED)	FSR 154
C		FSR 155
DO 23 J=1,200		FSR 156
23 JIN(J) = -1		FSR 157
C	READ AND PRINT INPUT DATA	FSR 158
C	GENERAL	FSR 159
C	I CARD READING	FSR 160
C	READ INPUT TAPE 2, 1001	FSR 161
C	J CARD READING	FSR 162
C	READ INPUT TAPE 2, 1006	FSR 163
C	K CARD READING	FSR 164
C	READ INPUT TAPE 2, 1001	FSR 165
9 NSER, IPDV, IPSFN, IPCFN, IPGFN, IPHFN, NOS, NEC, IPIGYN,		FSR 166
1 IPGTC, IPRL, IPNCI, IPJ, LAST		FSR 167
WRITE OUTPUT TAPE 3, 1010,		FSR 168
9 NSER		FSR 169
WRITE OUTPUT TAPE 3, 1001		FSR 170
9 NSER, IPDV, NOS, NEC, IPSFN, IPCFN		FSR 171
WRITE OUTPUT TAPE 3, 1011,		FSR 172
9 NSER, IPDV, IPJ, NOS, NEC, IPSFN, IPCFN		FSR 173
WRITE OUTPUT TAPE 3, 1012,		FSR 174
9 IPGFN, IPHEN, IPIGYN, IPGTC, IPRL, IPNCI		FSR 175
C	TEST FOR NO ENTRIES IN DATA SERIAL NUMBER INPUT LIST	FSR 176
C		FSR 177
IF ((IPSFN) 24,30,25		FSR 178
C	PAUSE REMOVED	FSR 179
24 CONTINUE		FSR 180
C	L CARD READING	FSR 181
C	READ INPUT TAPE 2, 1000,	FSR 182
9 (LSPN(K),K=1,IPSFN)		FSR 183
WRITE OUTPUT TAPE 3, 1013		FSR 184
WRITE OUTPUT TAPE 3, 1030,		FSR 185
9 (LSPN(K),K=1,IPSFN)		FSR 186
C	TEST FOR NO ENTRIES IN FUEL CLASS NUMBER INPUT LIST	FSR 187
C		FSR 188
30 IF ((IPCFN) 24,32,31		FSR 189
C	M CARD READING	FSR 190
C	READ INPUT TAPE 2, 1000,	FSR 191
9 (LCFN(K),K=1,IPCFN)		FSR 192
WHITE OUTPUT TAPE 3, 1014		FSR 193
		FSR 194
		FSR 195
		FSR 196
		FSR 197
		FSR 198
		FSR 199
		FSR 200
		FSR 201
		FSR 202
		FSR 203
		FSR 204
		FSR 205
		FSR 206
		FSR 207
		FSR 208

ROUTINE FSR	
(CONTINUED)	
FLAME SPEED REGRESSION CALCULATIONS	
WRITE OUTPUT TAPE 3, 1030, 9 (LCFNIK), K=1, IPGFN)	FSR 209 FSR 210
C TEST FOR NO ENTRIES IN FUEL CLASS-GROUP NUMBER INPUT LIST	FSR 211 FSR 212
C 32 IF (IPGFN) 24,34,33	FSR 213 FSR 214
C N CARD READING	FSR 215 FSR 216
C 33 READ INPUT TAPE 2, 1000, 9 (LGFN(1,K), LGFN(2,K), K=1, IPGFN)	FSR 217 FSR 218
WRITE OUTPUT TAPE 3, 1015	FSR 219 FSR 220
WRITE OUTPUT TAPE 3, 1040, 9 (LGFN(1,K), LGFN(2,K), K=1, IPGFN)	FSR 221 FSR 222
C TEST FOR NO ENTRIES IN FUEL CLASS-GROUP-MEMBER NUMBER INPUT LIST	FSR 223 FSR 224
C 34 IF (IPMFN) 24,40,35	FSR 225 FSR 226
C O CARD READING	FSR 227 FSR 228
C 35 READ INPUT TAPE 2, 1000, 9 (LMFN(1,K), LMFN(2,K), LMFN(3,K), K=1, IPMFN)	FSR 229 FSR 230
WRITE OUTPUT TAPE 3, 1016	FSR 231 FSR 232
WRITE OUTPUT TAPE 3, 1039, 9 (LMFN(1,K), LMFN(2,K), LMFN(3,K), K=1, IPMFN)	FSR 233 FSR 234
C TEST FOR NO ENTRIES IN CONTRIBUTOR TEST INPUT LIST	FSR 235 FSR 236
C 40 IF (IPIGTN) 24,55,41	FSR 237 FSR 238
C P CARD READING	FSR 239 FSR 240
C 41 READ INPUT TAPE 2, 1000, 9 (LIGTN(K)), LIGTN(K), K=1, IPIGTN)	FSR 241 FSR 242
WRITE OUTPUT TAPE 3, 1017	FSR 243 FSR 244
WRITE OUTPUT TAPE 3, 1031,	FSR 245 FSR 246
9 (LIGTN(K)), LIGTN(K), K=1, IPIGTN)	FSR 247
C SET UP COMPLETE LIST OF CONTRIBUTOR COUNT TEST NUMBERS	
C - 0 - OMIT	FSR 248
C - 1 - ACCEPT	FSR 249
C - 2 - REJECT GROUP IF COUNT NOT ZERO	FSR 250
C - 3 - REJECT GROUP IF COUNT ZERO	FSR 251
C - 4 TO 9 - CONDITIONAL TESTS	FSR 252
DO 48 K=1, IPIGTN	FSR 253
J1 = LIGTN(K)	FSR 254
IF (K = IPIGTN) 44,43,42	FSR 255
C PAUSE REMOVED	FSR 256
42 CONTINUE	FSR 257
C SET CONTRIBUTOR CODE NUMBER LIMIT	FSR 258
C 43 J2 = IPJ	FSR 259
GO TO 45	FSR 260
C REAJUST UPPER LIMIT TO NOT OVERLAP NEXT FIELD	FSR 261
C 44 J2 = LIGTN(K+1) - 1	FSR 262
C STORE CONTRIBUTOR COUNT TEST NUMBERS IN SEQUENCE	FSR 263
C 45 DO 48 J= J1,J2	FSR 264
LIGTN(J) = LIGTN(K)	FSR 265
IF (LIGTN(J)) 46,47,48	FSR 266
C PAUSE REMOVED	FSR 267
46 CONTINUE	FSR 268
47 JIN(J) = 0	FSR 269
48 CONTINUE	FSR 270
C TEST FOR NO ENTRIES IN CONDITIONAL TEST CRITERIA LIST	FSR 271
C 50 IF (IPCTC) 24,55,51	FSR 272
51 IPCTC3 = IPCTC + 3	FSR 273
C Q CARD READING	FSR 274
C READ INPUT TAPE 2, 1000, 9 (LCCTC(K), K=4, IPCTC3)	FSR 275
WRITE OUTPUT TAPE 3, 1018	FSR 276
WRITE OUTPUT TAPE 3, 1030, 9 (LCCTC(K), K=4, IPCTC3)	FSR 277
C SET UP ESSO REGRESSION CONTROL DATA	FSR 278
C INITIALIZE WITH STANDARD VALUES OF DECIMAL QUANTITIES	FSR 279
C 55 RCCL(1) = 0.001	FSR 280
RCCL(2) = 0.00002	FSR 281
RCCL(3) = 0.00001	FSR 282
C INITIALIZE WITH STANDARD VALUES OF INTEGER QUANTITIES	FSR 283
C DU 56 K=4,11	FSR 284
56 LNCC(1) = 1	FSR 285
LNCC(5) = 0	FSR 286
LNCC(10) = 0	FSR 287
C TEST FOR NO ENTRIES IN DECIMAL OVERRIDE LIST	FSR 288
C 57 IF (IPRCL) 24,58,57	FSR 289
C R CARD READING	FSR 290
C SUBSTITUTE OVERRIDING DECIMAL VALUES	FSR 291

## ROUTINE FSR

(CONTINUED)

## FLAME SPEED REGRESSION CALCULATIONS

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C   57 READ INPUT TAPE 2, 2001,
      9      (HCCL(K),K=1,3)          FSR 312
C   TEST FOR NO ENTRIES IN INTEGER OVERRIDE LIST    FSR 314
C   58 IF (IPLRC) 24,61,59                          FSR 315
C   59 S CARD HEADING                            FSR 316
C   60 READ INPUT TAPE 2, 1000,                   FSR 317
      9      (NRCK(K),LRC(K),K=1,IPLRC)        FSR 318
C   SUBSTITUTE OVERRIDING INTEGER VALUES          FSR 319
C   DO 60 K=1,IPLRC
      L = NRCK(K)                                FSR 320
      60 LRCC(K) = LRC(K)                         FSR 321
C   PRINTOUT OF ESSO REGRESSION CONTROL NUMBER LIST FSR 322
C   61 WRITE OUTPUT TAPE 3, 1019                  FSR 323
      WRITE OUTPUT TAPE 3, 1032,                   FSR 324
      9      (HCCL(K),K=1,3),(LRCC(K),K=4,11)     FSR 325
C   SET UP LIST OF DEPENDENT VARIABLE CODE NUMBERS AND NUMBER OF FSR 326
      CORRESPONDING PRESPECIFIED REGRESSION COEFFICIENTS FSR 327
C   65 DO 67 KDV = 1,IPDV                         FSR 328
C   66 T CARD READING                            FSR 329
C   HEAD INPUT TAPE 2, 1000,                      FSR 330
      9      LUVM(KDV),LDVD(KDV),LPGCC(KDV)       FSR 331
C   TEST FOR NO PRESPECIFIED REGRESSION COEFFICIENTS FSR 332
C   IF (LPGCC(KUV)) 24,67,66                      FSR 333
      66 IPGCC = LPGCC(KDV)                         FSR 334
C   U CARD ASSIGNMENTS                           FSR 335
C   660 CALL INPUT                               FSR 336
      M = 0                                         FSR 337
      LIMIT = 10+IC                                FSR 338
      IGO = LIMIT - 9                             FSR 339
      IF (LIMIT - IPGCC) 662, 662, 661           FSR 340
      661 LIMIT = IPGCC                           FSR 341
      662 DO 663 K = IGO, LIMIT                 FSR 342
      K = M + 1                                    FSR 343
      (GCCCNK,KUV) = INF(M)                      FSR 344
      663 GUC(K,KUV) = DEC(M)                    FSR 345
      IF (LIMIT - IPGCC) 660, 67, 67             FSR 346
      67 CONTINUE                                  FSR 347
C   START OF FIRST TAPE 6 PASS                  FSR 348
C   HEADING READING                            FSR 349
C   100 HEAD INPUT TAPE 6, 1002                FSR 350
C   INDIVIDUAL DATA GROUP READING            FSR 351
C   READ INPUT TAPE 6, 1003, IPI               FSR 352
      0111 = 1.0                                 FSR 353
      N = 0                                         FSR 354
      00 190 I-1,IPI                            FSR 355
      READ INPUT TAPE 6, 1004,                   FSR 356
      9      (SFN,FN1,FN2,LCFN,IGFN,IMFN,INDS,INEC,(D(K),K=2,6) FSR 357
      1 ,IPFGC,(FGCCN(K),FCCL(K),K=1,IPFGC)      FSR 358
C   TEST FOR DATA GROUP SERIAL NUMBER SEQUENCE FSR 359
C   IF (I - SFN) 104,106,104                  FSR 360
C   PAUSE REMOVED                            FSR 361
C   104 CONTINUE                                FSR 362
C   TEST FOR LIMIT OF 300 ACCEPTABLE DATA GROUPS FSR 363
C   106 IF (N-300) 110,107,105                FSR 364
C   PAUSE REMOVED                            FSR 365
C   107 PFAIL = 3.0                            FSR 366
      GO TO 190                                FSR 367
C   START TESTING SEQUENCE FOR ACCEPTABLE REGRESSION DATA FSR 368
C   110 IF ((PSFN) 111,120,112                FSR 369
C   PAUSE REMOVED                            FSR 370
C   111 CONTINUE                                FSR 371
C   TEST FOR UNACCEPTABLE DATA GROUP SERIAL NUMBERS FSR 372
C   112 DO 113 K = 1,IPSFN                   FSR 373
      IF (I - LSFN(K)) 113,190,113            FSR 374
      113 CONTINUE                                FSR 375
      120 IF ((PCPN) 111,123,121)              FSR 376
C   TEST FOR ACCEPTABLE FUEL CLASS NUMBER      FSR 377
C   121 DO 122 K=1,LCFN                      FSR 378
      IF ((LCFN - LCFN(K)) 122,123,122        FSR 379
      122 CONTINUE                                FSR 380
      GO TO 190                                FSR 381

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ROUTINE	FSR	(CONTINUED)
FLAME SPEED REGRESSION CALCULATIONS		
123 IF ((PGFN) 111,126,124	FSR 417	
C TEST FOR ACCEPTABLE FUEL CLASS-GROUP NUMBERS	FSR 418	
C	FSR 419	
124 DO 125 K=1,1PGFN	FSR 420	
IF ((CFN-LGPN(1,K)) 125,1241,125	FSR 421	
1241 IF ((LGPN-LGPN(2,K)) 125,126,125	FSR 422	
125 CONTINUE	FSR 423	
GO TO 190	FSR 424	
126 IF ((PMFN) 111,130,127	FSR 425	
C TEST FOR ACCEPTABLE FUEL CLASS-GROUP-MEMBER NUMBERS	FSR 426	
C	FSR 427	
127 DU 128 K=1,1PMFN	FSR 428	
IF ((CFN-LMFN(1,K)) 128,1271,128	FSR 429	
1271 IF ((CFN-LMFN(2,K)) 128,1272,128	FSR 430	
1272 IF ((LMFN-LMFN(3,K)) 128,190,128	FSR 431	
128 CONTINUE	FSR 432	
130 IF ((ND5) 111,135,131	FSR 433	
C TEST FOR ACCEPTABLE DATA SOURCE NUMBER	FSR 434	
C	FSR 435	
131 IF ((NDUS - ND5) 190,135,190	FSR 436	
135 IF ((NEC) 111,140,136	FSR 437	
C TEST FOR ACCEPTABLE EXPERIMENTAL CONDITIONS NUMBER	FSR 438	
C	FSR 439	
136 IF ((NEC - NEC) 190,140,190	FSR 440	
C TEST FOR AN UNDEFINED DEPENDENT VARIABLE	FSR 441	
C (UNACCEPTABLE IF EITHER NUMERATOR OR DENOMINATOR ZERO)	FSR 442	
C	FSR 443	
140 DU 142 KDV=1,1PDV	FSR 444	
K = LDVN(KDV)	FSR 445	
IF ((D(K)) 141,190,141	FSR 446	
141 K = LDVD(KDV)	FSR 447	
IF ((D(K)) 142,190,142	FSR 448	
142 CONTINUE	FSR 449	
150 IF ((PIGIN) 111,180,151	FSR 450	
C TEST FOR CONTRIBUTOR COUNT TESTS	FSR 451	
C	FSR 452	
151 DU 152 J=1,1PJ	FSR 453	
152 FGCI(J) = 0.0	FSR 454	
DJ 153 K=1,1PFGC	FSR 455	
J = LFUGCN(K)	FSR 456	
C STORE CONTRIBUTOR NUMBERS FROM GROUP BEING TESTED	FSR 457	
C	FSR 458	
153 FGCI(J) = FGCI(K)	FSR 459	
(H) 154 K=4,9	FSR 460	
NZ(K) = U	FSR 461	
154 NZ(K) = 0	FSR 462	
C OPERATIONS ON CONTRIBUTOR COUNT TEST NUMBERS	FSR 463	
C	FSR 464	
DO 165 J = 1,1PJ	FSR 465	
JGTM = LGTM(J)	FSR 466	
C CONTRIBUTOR COUNT TEST 2 - ONLY ZERO COUNTS ACCEPTED	FSR 467	
C	FSR 468	
IF (JGTM - 2) 165,156,157	FSR 469	
156 IF (FGCI(J)) 190,165,190	FSR 470	
C CONTRIBUTOR COUNT TEST 3 - ONLY NON-ZERO COUNTS ACCEPTED	FSR 471	
C CONTRIBUTOR COUNT TESTS 4 TO 9	FSR 472	
C	FSR 473	
157 IF (JGTM - 3) 158,159,160	FSR 474	
C PAUSE REMOVED	FSR 475	
158 CONTINUE	FSR 476	
159 IF (FGCI(J)) 165,190,165	FSR 477	
160 IF (FGCI(J)) 161,162,161	FSR 478	
C SUM OF NON-ZERO VALUES OF INDEX (JGTM)	FSR 479	
C	FSR 480	
161 NNZ(JGTM) = NZ(JGTM) + 1	FSR 481	
GO TO 165	FSR 482	
C SUM OF ZERO VALUES OF INDEX (JGTM)	FSR 483	
C	FSR 484	
162 NZ(JGTM) = NZ(JGTM) + 1	FSR 485	
165 CONTINUE	FSR 486	
IF ((WCIC) 111,180,171	FSR 487	
C TEST FOR CONDITIONAL CONTRIBUTOR COUNT TESTS	FSR 488	
C	FSR 489	
171 DO 175 K=4,1PCTC3	FSR 490	
IF ((LCTC(K)) 172,175,173	FSR 491	
172 IF ((NZ(K)) + LCTC(K)) 190,175,175	FSR 492	
173 IF ((NNZ(K)) - LCTC(K)) 190,175,175	FSR 493	
175 CONTINUE	FSR 494	
C CALCULATIONS ON ACCEPTABLE DATA GROUPS	FSR 495	
C	FSR 496	
180 DU 182 K=1,1PFGC	FSR 497	
J = LFUGCN(K)	FSR 498	
C JIN(J) EITHER -1 OR 0	FSR 499	
C	FSR 500	
IF ((JIN(J) + 1) 182,181,182	FSR 501	
181 JIN(J) = 1	FSR 502	
182 CONTINUE	FSR 503	
N = N + 1	FSR 504	
LORSFR(N) = 1	FSR 505	
C	FSR 506	
FSR 507	FSR 508	
FSR 508	FSR 509	
FSR 509	FSR 510	
FSR 510	FSR 511	
FSR 511	FSR 512	
FSR 512	FSR 513	
FSR 513	FSR 514	
FSR 514	FSR 515	
FSR 515	FSR 516	
FSR 516	FSR 517	
FSR 517	FSR 518	
FSR 518	FSR 519	
FSR 519	FSR 520	

ROUTINE	FSK	(CONTINUED)
FLAME SPEED REGRESSION CALCULATIONS		
C		
C	SETUP OF DESIRED DEPENDENT VARIABLE	FSR 521
C	DO 189 KDV = 1,IPDV	FSK 522
C	KDVM = LDVN(KDV)	FSR 523
C	KDVO = LDVO(KDV)	FSR 524
C	Y = D(KDV)/D(KDV)	FSR 525
C	IPCGC = L(IPGCC(KDV))	FSR 526
C		FSR 527
C		FSR 528
C		FSR 529
C	TEST FOR NU PRESPECIFIED COEFFICIENTS	FSR 530
C	IF (IPGCC) 111,189,184	FSR 531
184	DO 188 K=1,IPFGC	FSR 532
	J = LGCCN(K)	FSR 533
C	TEST ONLY THOSE CONTRIBUTOR WHICH ARE NOT TO BE OMITTED	FSR 534
C	IF (JINI(J) = 1) 188,185,188	FSR 535
185	DO 186 L=1,IPGCC	FSR 536
C	TEST EACH CONTRIBUTOR IN GROUP	FSR 537
C	IF (J = LGCCN(L,KDV)) 186,187,186	FSR 538
186	CONTINUE	FSR 539
	GO TO 188	FSR 540
C	ADJUST VALUE OF DEPENDENT VARIABLE	FSR 541
C	187 Y = Y - CGC(L,KDV)+FGCL(K)	FSR 542
188	CONTINUE	FSR 543
C	DETERMINE MAXIMUM VALUE OF Y FOR SCALING TO FIT ESSO OUTPUT	FSR 544
C	189 YMIX(KDV) = MAX(YMX(KDV),ABSF(Y))	FSR 545
C	FN1(L) = FN1	FSR 546
C	FN2(L) = FN2	FSR 547
190	CONTINUE	FSR 548
C	IPN = N	FSR 549
C	READ INPUT TAPE 6, 1005, (GNL(J),J=1,200)	FSR 550
C	READ INPUT TAPE 6, 1005, (DNM(K)),K=1,6)	FSR 551
C	REWIND 6	FSR 552
C		FSR 553
C	END OF FIRST TAPE 6 PASS	FSR 554
C		FSR 555
C	TEST FOR NO ACCEPTABLE DATA	FSR 556
C	IF (IPN) 191,191,192	FSR 557
C	DIAGNOSTIC - NO DATA ACCEPTABLE - PROCESS NEXT RUN	FSR 558
C	191 WRITE OUTPUT TAPE 3, 1025	FSR 559
C	GO TO 302	FSR 560
C		FSR 561
C	PRINT LIST OF ACCEPTABLE DATA SERIAL NUMBER AND FUEL NAMES	FSR 562
C	192 LKCC(3) = IPN	FSR 563
C	WRITE OUTPUT TAPE 3, 1022	FSR 564
193	WRITE OUTPUT TAPE 3, 1034,	FSR 565
	9 (LOKSFN(N), FN1(N), FN2(N), N=1, IPN)	FSR 566
C	TEST FOR DIAGNOSTIC PRINTOUT - FIRST 300 DATA GROUPS USED	FSR 567
C	IF (PFAIL = 3.0) 200,194,200	FSR 568
194	WRITE OUTPUT TAPE 3, 1027	FSR 569
C	PFAIL = 0.0	FSR 570
C	GENERATION OF ESSO REGRESSION INPUT DATA	FSR 571
C	SET UP DEPENDENT VARIABLE	FSR 572
C	200 DU 300 KDV=1,IPDV	FSR 573
C	KDVM = LDVN(KDV)	FSR 574
C	KDVO = LDVO(KDV)	FSR 575
C	IPGCC = L(IPGCC(KDV))	FSR 576
C	IF (IPGCC) 24,210,206	FSR 577
206	DO 207 J=1,IPJ	FSR 578
207	CGC(J,J) = 0.0	FSR 579
C	SET UP LIST OF PRESPECIFIED COEFFICIENTS	FSR 580
C	UD 204 K = 1,IPGC	FSR 581
C	J = LGCCN(K,KDV)	FSR 582
C	CGC(J,J) = CGC(K,KDV)	FSR 583
C	IF (JINI(J) = 1) 204,208,209	FSR 584
C	SET JINI(J) = 2 FOR CONTRIBUTOR WITH SPECIFIED COEFFICIENTS ONLY	FSR 585
C	208 JINI(J) = 2	FSR 586
209	CONTINUE	FSR 587
C	DETERMINE NUMBER OF INDEPENDENT VARIABLES FOR REGRESSION	FSR 588
C	210 M = 0	FSR 589
C	MC = 0	FSR 590
C	DU 213 J=1,IPJ	FSR 591
C	IEST FOR STATUS OF CONTRIBUTOR	FSR 592
C	IF (JINI(J) = 1) 213,211,212	FSR 593
C	INCREMENT NUMBER OF DEPENDENT VARIABLES INDEX	FSR 594
C	211 N = N + 1	FSR 595
C	LIVCN(M) = J	FSR 596

ROUTINE FSR	
(CONTINUED)	
FLAME SPEED REGRESSION CALCULATIONS	
GML(M) = GML(J)	FSR 625
GO TO 213	FSR 626
C INCREMENT NUMBER OF PRESPECIFIED COEFFICIENTS INDEX	FSR 627
C 212 MC = MC + 1	FSR 628
C GCGNL(MC) = GML(J)	FSR 629
C LCCCN(MC) = J	FSR 630
C 213 CONTINUE	FSR 631
IPH = MC	FSR 632
IPMC = MC	FSR 633
C TEST FOR EXCEEDING LIMIT OF DEPENDENT VARIABLES COUNT OF ESSO	FSR 634
C REGRESSION PROGRAM	FSR 635
C IF (IPH-57) 220,220,216	FSR 636
216 PFAIL = 1.0	FSR 637
GO TO 260	FSR 638
C FINAL MAKEUP OF ESSO REGRESSION CONTROL DATA	FSR 639
C 220 LRCC(1) = KDV	FSR 640
LRCC(2) = IPH + 1	FSR 641
LHCC(3) = IPN	FSR 642
C WRITE TITLE AND CONTROL DATA FOR REGRESSION ANALYSIS	FSR 643
C 221 WRITE OUTPUT TAPE 7, 1006	FSR 644
WRITE OUTPUT TAPE 7, 1007, (RCCL(K),K=1,3), (LRCC(K),K=1,3)	FSR 645
C START OF SECOND TAPE 6 PASS	FSR 646
C READ INPUT TAPE 6, 1002	FSR 647
READ INPUT TAPE 6, 1003, IP1	FSR 648
C CALCULATION OF DEPENDENT VARIABLE SCALE FACTOR	FSR 649
C KSFE = 0	FSR 650
C REDUCE POWER OF 10 UNTIL YMX LESS THAN 1000.	FSR 651
C 221 IF (YMX(KDV)) = 1000.1 223,222,222	FSR 652
222 YMX(KDV) = YMX(KDV)/10.0	FSR 653
KSFE = KSFE + 1	FSR 654
GO TO 221	FSR 655
C INCREASE POWER OF 10 UNTIL YMX GREATER THAN 100.	FSR 656
C 223 IF (YMX(KDV)) = 100.01 224,230,230	FSR 657
224 KSFE = KSFE - 1	FSR 658
YMX(KDV) = 10.0*YMX(KDV)	FSR 659
GO TO 223	FSR 660
C CHOOSE ACCEPTABLE DATA GROUPS FROM TAPE	FSR 661
C 230 DO 255 N = 1,IPN	FSR 662
231 READ INPUT TAPE 6, 1004,	FSR 663
I, ISFN, FN1, FN2, ICFN, IGFN, IFNFN, INDS, INEC, IQ(K), K=2,6	FSR 664
I, IPFGC, (LFGCCN(K)), FGCL(K), K=1,1(PFGC)	FSR 665
C TEST FOR ACCEPTABLE SERIAL NUMBERS	FSR 666
C IF (ISFN = LUKSFN(N)) 231,235,232	FSR 667
C PAUSE REMOVED	FSR 668
232 CONTINUE	FSR 669
235 DO 236 J = 1,IPJ	FSR 670
236 FCCJ(J) = 0.0	FSR 671
DO 237 K = 1,IPFGC	FSR 672
J = LFGCCN(K)	FSR 673
237 FCCJ(J) = FGCL(K)	FSR 674
C PREPARE LIST OF INDEPENDENT CONTRIBUTOR COUNTS	FSR 675
C DO 238 N = 1,IPM	FSR 676
J = LIVCN(M)	FSR 677
238 OPL(N) = FCCJ(J)	FSR 678
C CALCULATION OF DEPENDENT VARIABLE	FSR 679
C 240 Y = D(RKDVN)/D(RKDV)	FSR 680
C TEST FOR NO PRESPECIFIED COEFFICIENTS	FSR 681
C IF (IPMC) 241,250,242	FSR 682
C PAUSE REMOVED	FSR 683
241 CONTINUE	FSR 684
242 DO 243 MC = 1,IPMC	FSR 685
J = LCCCN(MC)	FSR 686
C DEPENDENT VARIABLE ADJUSTMENT FROM PRESPECIFIED COEFFICIENTS	FSR 687
C 243 Y = Y - CGCJ(J)*FCCJ(J)	FSR 688
C DEPENDENT VARIABLE SCALING	FSR 689
C 250 Y = Y*10.0*(-KSFE)	FSR 690
C WRITE DATA FOR REGRESSION ANALYSIS	FSR 691
C 251 WRITE OUTPUT TAPE 7, 1006, ISFN, (OPL(N),N=1,IPM),Y	FSR 692
255 CONTINUE	FSR 693
REWIND 6	FSR 694
C END OF SECOND TAPE 6 PASS	FSR 695

## ROUTINE FSH

(CONTINUED)

## FLAME SPEED REGRESSION CALCULATIONS

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C      PRINTOUT OF SUCCESSFUL DATA PREPARATION INFORMATION          FSR 729
C      260 WRITE OUTPUT TAPE 3, 1010,                                     FSR 730
C          4 NSER,                                                 FSR 731
C          9 KDV,                                                 FSR 732
C          9 WRITE OUTPUT TAPE 3, 10101,                                     FSR 733
C          9 KSFE, DMN1(KDVN1), DMN1(KDV)                                FSR 734
C          IF (IPCGC) 24,262,261                                         FSR 735
C      261 WRITE OUTPUT TAPE 3, 1021,                                     FSR 736
C          9 IPMC,                                                 FSR 737
C          9 WRITE OUTPUT TAPE 3, 1033,                                     FSR 738
C          9 (LCGCN1(K,DKV), CGC1(K,DKV), K=1, IPCGC)                  FSR 739
C      C TEST FOR NO INDEPENDENT VARIABLES                            FSR 740
C      262 IF (IPM) 270,270,263                                         FSR 741
C      C PRINTOUT OF INDEPENDENT CONTRIBUTORS WITH THEIR REGRESSION   FSR 742
C          INDICES,                                               FSR 743
C      263 WRITE OUTPUT TAPE 3, 1023,                                     FSR 744
C          WRITE OUTPUT TAPE 3, 1035,                                     FSR 745
C          9 (NOL(K), K=1,10) .                                         FSR 746
C      C PRINT OUT FIRST 9                                           FSR 747
C      M2 = XMINOF(Y1,IPM)                                         FSR 748
C      WRITE OUTPUT TAPE 3, 1036,                                     FSR 749
C          9 (LIVCN(M), DGNL(M), M=1,M2)                                FSR 750
C          IF (IPM - 9) 270,270,265                                         FSR 751
C      265 LNX = IPH/10                                         FSR 752
C      C PRINT OUT IN SEQUENCES OF 10                               FSR 753
C      DD 266 LNX = 1,LNX                                         FSR 754
C      M1 = 10*LNX                                         FSR 755
C      M2 = XMINOF (M1+9,IPM)                                         FSR 756
C      266 WRITE OUTPUT TAPE 3, 1037,                                     FSR 757
C          9 M1,(LIVCN(M), DGNL(M), M=M1,M2)                                FSR 758
C      270 IF (IPMC) 280,280,271                                         FSR 759
C      C PRINTOUT OF NAMES OF CONTRIBUTORS WHICH HAVE PRESPECIFIED    FSR 760
C          COEFFICIENTS,                                              FSR 761
C      271 WRITE OUTPUT TAPE 3, 1024,                                     FSR 762
C          LN1 = 1 + (IPMC - 1)/10                                         FSR 763
C          DO 272 LN=1,LNX                                         FSR 764
C          M1 = 10*LN                                         FSR 765
C          M2 = XMINOF (M1+9,IPMC)                                         FSR 766
C      272 WRITE OUTPUT TAPE 3, 1038,                                     FSR 767
C          9 (LCGN(MC), DCGN(IPMC), MC=M1,M2)                                FSR 768
C      280 IF (PFAIL - 1.0) 290,281,290                                         FSR 769
C      C DIAGNOSTIC - CAPACITY OF REGRESSION ROUTINE EXCEEDED        FSR 770
C      281 WRITE OUTPUT TAPE 3, 1026,                                     FSR 771
C          PFFAIL = 0.0,                                              FSR 772
C          GO TO 2901,                                              FSR 773
C      290 PFFAIL = 0.0,                                              FSR 774
C          REWIND 7,                                              FSR 775
C      C INTAPE = 7,                                              FSR 776
C      CALL ESSO REGRESSION PROGRAM,                                     FSR 777
C      CALL ESSO4 ( INTAPE)                                         FSR 778
C      2901 DD 300 J= 1, IPJ                                         FSR 779
C      IF (JINI(J) - 2) 300,292,291                                         FSR 780
C      C PAUSE REMOVED,                                              FSR 781
C      291 CONTINUE,                                              FSR 782
C      292 JINI(J) = 1,                                              FSR 783
C      300 CONTINUE,                                              FSR 784
C      C TEST FOR END OF CALCULATIONS,                                     FSR 785
C      L 302 IF(ILAST)301,20,301                                         FSR 786
C      301 REWIND 7,                                              FSR 787
C      REWIND 6,                                              FSR 788
C      WRITE OUTPUT TAPE 3, 2000,                                         FSR 789
C      GO TO 20,                                              FSR 790
C      C FORMAT STATEMENTS,                                         FSR 791
C      1000 FORMAT ( 1B14)                                         FSR 792
C      1001 FORMAT (72H)                                         FSR 793
C          1                                         FSR 794
C      1002 FORMAT (72M)                                         FSR 795
C          1                                         FSR 796
C      1003 FORMAT (1H0 6I6 )                                         FSR 797
C      1004 FORMAT' 9 (1H0 2X6,5I6,1P5E12.4,16/(1H 16,E12.4,I6,E12.4,I6,     FSR 798
C          1E12.4,I6,E12.4,16,E12.4))                                FSR 799
C      1005 FORMAT' 9 (1H0 9(6X,A6,6X,A6,6X,A6,6X,A6,6X,A6,6X,A6,6X,     FSR 800
C          1A6,6X,A6))                                FSR 801
C      1006 FORMAT (72H)                                         FSR 802
C          1                                         FSR 803
C      1007 FORMAT ( 3F10.5,3I9,13,7I2)                                FSR 804
C      1008 FORMAT ( 17,5X,1P5E12.4 / (16E12.4))                      FSR 805
C      1010 FORMAT' 9 (1H1 3X, 48MMONSANTO RESEARCH CORPORATION FLAME SPEED REGRESSTO   FSR 806
C          IN - ROUTINE 1922 - MODIFICATION 1 - RUN 14)                   FSR 807
C      10101 FORMAT' 1                                         FSR 808

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## ROUTINE FSR

(CONTINUED)

## FLAME SPEED REGRESSION CALCULATIONS

9 (IH+, 107K UNPROBLEM 14 )	FSR 833
1011 FORMAT(1H0\$15\$RUN 14,17X 32HNUMBER OF PROBLEMS IN THIS RUN 14,	FSR 834
1 7X, 30HIGHEST CONTRIBUTOR CODE NUMBER IN USE 17 /	FSR 835
2 IH0 20X, 31HACCEPTABLE DATA SOURCE NUMBER 15,	FSR 836
3 7X, 33HACCEPTABLE EXPERIMENTAL CONDITIONS NUMBER 14 /	FSR 837
4 IH0 37X, 44HENTRIES TO BE READ FROM THE INPUT DATA CARDS /	FSR 838
5 IH0 3X, 9MCARD TYPE 3X, 17HNUMBER OF ENTRIES	FSR 839
6 20X, 17HLIST SIGNIFICANCE /	FSR 840
7 IH0 6X, 3H-L 14X,14, 8X, 40H- UNACCEPTABLE DATA GROUP SERIA	FSR 841
8L NUMBERS /	FSR 842
9 IH , 6X, 3H-N- 14X,14, 8X,31H- ACCEPTABLE FUEL CLASS NUMBERS /	FSR 843
1012 FORMAT	FSR 844
9 IH , 6X, 3H-N- 14X,14, 8X, 37H- ACCEPTABLE FUEL CLASS-GROUP NU	FSR 845
1MERS /1H ,6X,3H-O- 14X,14,8X, 40H- UNACCEPTABLE FUEL-CLASS-GROUP-	FSR 846
2MEMBER NUMBERS /	FSR 847
3 IH , 6X, 3H-P- 14X,14, 8X, 32H- CONTRIBUTOR COUNT TEST NUMBERS	FSR 848
4/ IH , 6X, 3H-U- 14X,14, 8X, 34H- CONDITIONAL COUNT TEST CRITERI	FSR 849
5A /IH , 6X, 3H-R- 14X,14, 8X, 44H- OVERRIDING DECIMAL REGRESSION	FSR 850
6CONTROL DATA /	FSR 851
7 IH , 6X, 3H-S- 14X,14, 8X, 44H- OVERRIDING INTEGER REGRESSION	FSR 852
8CONTROL DATA /	FSR 853
1013 FORMAT	FSR 854
9 (IH+, 10X, 46HLIST OF UNACCEPTABLE DATA GROUP SERIAL NUMBERS /)	FSR 855
1014 FORMAT	FSR 856
9 (IH0, 10X, 37HLIST OF ACCEPTABLE FUEL CLASS NUMBERS /)	FSR 857
1015 FORMAT	FSR 858
9 (IH0, 10X, 43HLIST OF ACCEPTABLE FUEL CLASS-GROUP NUMBERS /)	FSR 859
1016 FORMAT	FSR 860
9 (IH0, 10X, 52HLIST OF UNACCEPTABLE FUEL CLASS-GROUP-MEMBER NUMBER	FSR 861
IS /)	FSR 862
1017 FORMAT	FSR 863
9 (IH0, 10X, 31HLIST OF CONTRIBUTOR COUNT TESTS /)	FSR 864
1018 FORMAT	FSR 865
9 (IH0, 10X, 27HLIST OF COUNT TEST CRITERIA /)	FSR 866
1019 FORMAT	FSR 867
9 (IH0, 10X, 24HESO REGRESSION CONTROL LIST /)	FSR 868
1020 FORMAT	FSR 869
9 (IH0, 6BX, 13 /	FSR 870
1 IH ,10X, 21HDEPENDENT VARIABLE = A6,1H/ A6, 4H X10 )	FSR 871
1021 FORMAT	FSR 872
9 (IH0,10X, 6HMINUS 14, 32H CONTRIBUTIONS OF THE FOLLOWING /	FSR 873
1 IH ,10X,69HLIST OF CONTRIBUTOR CODE NUMBERS WITH THEIR PRESPECIF	FSR 874
2IED COEFFICIENTS /)	FSR 875
1022 FORMAT	FSR 876
9 (IH0, 10X, 51HLIST OF ACCEPTED DATA SERIAL NUMBERS AND FUEL NAMES	FSR 877
1 / /	FSR 878
1023 FORMAT	FSR 879
9 (IH0, 10X, 77HLIST OF INDEPENDENT CONTRIBUTORS WITH THEIR CORRESP	FSR 880
ONDING REGRESSION INDICIES /)	FSR 881
1024 FORMAT	FSR 882
9 (IH0, 10X, 53HLIST OF CONTRIBUTORS HAVING PRESPECIFIED COEFFICIENT	FSR 883
115 / /	FSR 884
1025 FORMAT	FSR 885
9 (IH0, 10X, 18HNO ACCEPTABLE DATA )	FSR 886
1026 FORMAT	FSR 887
9 (IH0, 10X, 39HCAPACITY OF REGRESSION ROUTINE EXCEEDED )	FSR 888
1027 FORMAT	FSR 889
9 (IH0, 10X, 46HONLY THE FIRST 300 ACCEPTABLE DATA GROUPS USED )	FSR 890
1030 FORMAT	FSR 891
9 (IH , 10X, 1816)	FSR 892
1031 FORMAT	FSR 893
9 (IH , 10X, 16,13,16,13,16,13,16,13,16,13,16,13,16,13,	FSR 894
116,13,16,13,16,13 )	FSR 895
1032 FORMAT	FSR 896
9 (IH , 10X, 3(F10.5,3X), 10X, 14, 7(3.)	FSR 897
1033 FORMAT	FSR 898
9 (IH , 11X, 16,1PE12.4, 16,E12.4, 16,E12.4, 16,E12.4,	FSR 899
1 16,E12.4 )	FSR 900
1034 FORMAT	FSR 901
9 (IH , 11X, 15,1X,246,15,1X,246, 15,1X,246, 15,1X,246,	FSR 902
1 15,1X,246, 15,1X,246 )	FSR 903
1035 FORMAT	FSR 904
9 (IH , 5X, 19, 9111)	FSR 905
1036 FORMAT	FSR 906
9 (IH , 20X, 9114,1X,A61)	FSR 907
1037 FORMAT	FSR 908
9 (IH , 12,7X,10(I4,1X,A61))	FSR 909
1038 FORMAT	FSR 910
9 (IH , 9X, 10(I4,1X,A61))	FSR 911
1039 FORMAT	FSR 912
9 (IH , 10X, 14,3H / 12, 18,3H / 12, 18,3H / 12,	FSR 913
1 18,3H / 12,3H / 12, 18,3H / 12,3H / 12,	FSR 914
2 18,3H / 12,3H / 12, 18,3H / 12,3H / 12 )	FSR 915
1040 FORMAT	FSR 916
9 (IH , 10X, 14,3H / 12, 18,3H / 12, 18,3H / 12,	FSR 917
1 18,3H / 12,3H / 12, 18,3H / 12,3H / 12,	FSR 918
2 18,3H / 12,3H / 12, 18,3H / 12,3H / 12 )	FSR 919
2000 FORMAT(1H0, 25X, 20HEXECUTION COMPLETED )	FSR 920
2001 FORMAT( 3F10.5 )	FSR 921
END	

**SUBROUTINE ESS04**

## MULTIPLE LINEAR REGRESSION CALCULATIONS

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* LIST0
* SYMBOL TABLE
C ESS002 ESS00 ESS00 REGRESSION SUBROUTINE MOD 4
C PRESPECIFIU INPUT FORMAT OF 12.3
C VARIABLE INPUT TAPE SPECIFICATIONS
C SUBROUTINE ESS004 ( INTAPE)
DIMENSION DATA(60),VECT0(60,60),AVE(60),SIGMA(60),COEN(60),SIGNCO
1(60),INDEX(60)
DIMENSION RATIO(60) ,DEC(101), FMT(120) , HEAD(12)
REWIND INTAPE
READ INPUT TAPE INTAPE, 4000,(HEAD(I), I=1,12)
READ INPUT TAPE INTAPE, 5,
      9, TOL, EFIN,EFOUT,NOPR0B,INVAR,NODATA,IFMT,IPSTEP
1,IFRAW,IFAVE,IFRESD,IFCOEN,IPRED,IFCNST
INDATA = 1
NRNUN = 1
IDEPS0 = INVAR + 1
IWEIGT = INVAR + 2
GO TO 1,101,102,INDATA
101 WRITE OUTPUT TAPE 3, 5003,(HEAD(I), I = 1, 12)
WRITE OUTPUT TAPE 3,
      9, 6, TOL, EFIN,EFOUT,NOPR0B,INVAR,NODATA,IFMT,IPSTEP
1,IFRAW,IFAVE,IFRESD,IFCOEN,IPRED,IFCNST
102 DO 4020 I=1,INVAR
4020 CNIEN(I)=0.0
C IFMT = 1, THEN ALL WHTS = 1.0
C IPSTEP = 1, DO NOT PRINT EACH STEP
C IFRAW = 1, DO NOT PRINT RAW SUMS AND SQUARES
C IFAVE = 1, DO NOT PRINT AVERAGES
C IFRESD = 1, DO NOT PRINT RESIDUAL SUMS SQUARES
C IFCOEN = 1, DO NOT PRINT PARTIAL COEFFICIENTS
C IPRED = 1, DO NOT CALC PREDICTED VALUES
C IFCNST = 1, DO NOT HAVE CONST TERM IN EQUATION
C INDATA = 1, LIST INPUT DATA ON TAPE 3
NODIN = 0
VAR = 0
K = 0
LEVEL = 0
NUENT = 0
NDMIN = 0
NUMAX = 0
NOVAR = INVAR
NPV1 = NOVAR + 1
110 DO 120 I = 1, NPV1
120 DO 120 J = 1, NPV1
120 VECT0(I,J) = 0.0
121 REWIND 8
140 IF(IFWEI) 900, 500, 150
900 WRITE OUTPUT TAPE 3, 905
GO TO 910
150 INPUT = NOVAR + 1
DO 170 N = L, NODATA
160 READ INPUT TAPE INTAPE,5000, (DEC(I), I = 1, INPUT )
J1 = I
RUN = DEC(INKUNSE)
DATA1(NOVAR) = DEC(IDEPS0)
DO 1613 J=1, INPUT
1F1 J - NRNUNSE1(1611,1613,1611
1611 IF1 J - IDEPS01(1612,1613,1612
1612 DATA1(J1) = DEC(J)
J1 = J1 + 1
1613 CONTINUE
161 WRITE TAPE 8,(DATA1(L), L = 1, NOVAR),RUN
GO TO 1,162,180,INDATA
162 WRITE OUTPUT TAPE 3,
      9, 11, RUN, ( DATA1(L) , L = 1, NOVAR )
180 DO 190 I = 1, NOVAR
200 VECTOR(I,) ,NOVAR + 1) = VECTOR(I, NOVAR + 1) + DATA(I)
210 DO 220 J = 1, NOVAR
220 VECTOR (I,J) = VECTOR(I,J) + DATA(I) * DATA(J)
190 CONTINUE
170 VECTOR(NPV1, NPV1) = VECTOR(NPV1, NPV1) + 1.0
230 GO TO 562
C CALCULATION SUMS WHEN VARIABLE WEIGHTS
500 INPUT = NOVAR + 2
DO 510 N = 1, NODATA
520 READ INPUT TAPE INTAPE,5000, (DEC(I), I = 1, INPUT )
J1=1
RUN = DEC(INKUNSE)
DATA1(NOVAR) = DEC(IDEPS0)
WHT = DEC(IWEIGT)
DO 5204 J=1, INPUT
1F1 J - NKUNSE1(5201, 5204, 5201
5201 IF1 J - IDEPS01(5202, 5204, 5202
5202 IF1 J - IWE(GT) 5203, 5204, 5203
5203 DATA1(J1) = DEC(J)
J1 = J1 + 1
5204 CONTINUE
521 WRITE TAPE 8,(DATA1(L), L = 1, NOVAR),RUN
GO TO 1,522,530,INDATA
522 WRITE OUTPUT TAPE 3,
      9, 11, RUN, ( DATA1(L) , L = 1, NOVAR )
530 DO 540 I = 1, NOVAR
550 VECTOR (I,NOVAR + 1) = VECTOR (I, NOVAR + 1) + DATA (I) * WHT
560 DO 540 J = 1, NOVAR
540 VECTOR (I,J) = VECTOR (I, J) + DATA (I) * DATA (J) * WHT
510 VECTOR (NPV1, NPV1) = VECTOR (NPV1, NPV1) + WHT
C COMPLETED SUMS OF SQUARES AND CROSS PRODUCTS. THESE ARE IN
C 1ST POSITION IN LOCATION VECTOR (I, J). THESE WILL BE PRINTED OUT ON
C 2TAPE 3 UNDER CONTROL OF STATEMENT 100
565 NOVNL = NOVAR - 1
566 NOVPL = NOVAR + 1
REWIND INTAPE
WRITE OUTPUT TAPE 3, 5003,(HEAD(I), I = 1, 12)

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## SUBROUTINE ESS04

(CONTINUED)

## MULTIPLE LINEAR REGRESSION CALCULATIONS

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567 WRITE OUTPUT TAPE 3, 90, NOPHOB, NODATA, NOVAR, VECTOR(NOVPL),  

  NOVPL, EFIN, EFOUT  

570 GO TO 4003  

4003 IF(IFRAME) 900,580,650  

580 WRITE OUTPUT TAPE 3, 15  

590 WRITE OUTPUT TAPE 3, 20, II, VECTOR (II, NOVPL), I = 1, NOVM1  

600 WRITE OUTPUT TAPE 3, 25, VECTOR (NOVAR, NOVPL)  

610 WRITE OUTPUT TAPE 3, 30  

620 WRITE OUTPUT TAPE 3, 35, II, J, VECTOR(II, NOVM1), J=1, NOVM1  

630 WRITE OUTPUT TAPE 3, 40, II, VECTOR(II, NOVAR), I=1, NOVM1  

640 WRITE OUTPUT TAPE 3, 45, VECTOR (NOVAR, NOVAR)  

650 GO TO 650  

C  CALCULATION OF RESIDUAL SUMS OF SQUARES AND CROSS PRODUCTS  

650 IF(IFCNST) 900,651,735  

651 IF(VECTOR(NOVPL,NOVPL)) 652,652,655  

652 WRITE OUTPUT TAPE 3, 654  

653 GO TO 910  

655 DO 660 I = 1, NOVAR  

656 DO 660 J = 1, NOVAR  

660 VECTOR (I,J) = VECTOR (I,J) - VECTOR(I,NOVPL) * VECTOR (J,NOVPL)  

   - / VECTOR (NOVPL, NOVPL)  

660 DU 660 I = 1, NOVAR  

660 AVE (I) = VECTOR(I,NOVPL) / VECTOR(NOVPL,NOVPL)  

700 IF (IIFAVE) 900, 710, 735  

710 WRITE OUTPUT TAPE 3, 50  

720 WRITE OUTPUT TAPE 3, 20, II, AVE(I), I = 1, NOVM1  

730 WRITE OUTPUT TAPE 3, 25, AVE(NOVAR)  

735 IF (IIPRESD) 900, 740, 780  

740 WRITE OUTPUT TAPE 3, 55  

750 WRITE OUTPUT TAPE 3, 35, II, J, VECTOR(II, J), J=I, NOVM1, I=1, NOVM1  

760 WRITE OUTPUT TAPE 3, 40, II, VECTOR(II, NOVAR), I=1, NOVM1  

770 WRITE OUTPUT TAPE 3, 45, VECTOR(NOVAR,NOVAR)  

780 NOSTEP = -1  

781 ASSIGN 1320 TO NUMBER  

782 DEFR = VECTOR(NOVPL,NOVPL) - 1.0  

790 DU 800 I = 1,NOVAR  

791 IF(VECTOR(I,I)) 792,794,810  

792 WRITE OUTPUT TAPE 3, 793  

9      1  

   GO TO 910  

793 FORMAT (3IH ERROR RESIDUAL SQUARE VARIABLE 14,31H IS NEGATIVE,PROB  

ILEN TERMINATED )  

794 WRITE OUTPUT TAPE 3,795, 1  

795 SIGMA(II) = 1.0  

797 GO TO 800  

798 FORMAT(1H0) VARIABLE 15,12H IS CONSTANT )  

810 SIGMA(II) = SQRT (VECTOR (I,I))  

800 VECTOR (I,I) = 1.0  

820 DU 830 I = 1,NOVM1  

840 DU 830 J = I, NOVAR  

841 DU 830 J = I, NOVAR  

850 VECTOR(I,J) = VECTOR(I,J) / SIGMA(II)* SIGMA(JJ)  

850 VECTOR(I,J) = VECTOR(I,J)  

860 IF (IFCDEN) 900, 870, 1000  

870 WRITE OUTPUT TAPE 3, 60  

874 NOVM2 = NOVM1 - 1  

875 DU 885 I = 1, NOVM2  

880 IPI = I + 1  

882 WRITE OUTPUT TAPE 3, 35, II, J, VECTOR(I,J), J= (IPI,NOVM1 )  

890 WRITE OUTPUT TAPE 3, 40, II, VECTOR(II, NOVAR), I=1, NOVM1  

1000 NOSTEP = NOSTEP + 1  

1001 IF (VECTOR(II, NOVAR,NOVAR)) 1002,1002,1010  

1002 NSTPM1 = NOSTEP - 1  

1003 WRITE OUTPUT TAPE 3, 1004, NSTPM1  

GO TO 1381  

1010 SIGY = SIGMAIN(NOVAR) * SQRT (VECTOR(NOVAR,NOVAR)/ DEFR)  

1015 DEFR = DEFR-1.0  

1016 IF (DEFR ) 1017,1017, 1020  

1017 WRITE OUTPUT TAPE 3, 1019, NOSTEP  

   GO TO 1381  

1020 VMIN = 0.0  

1030 VMAX = 0.0  

1035 NOMIN = 0  

1040 DO 1050 I = 1,NOVM1  

1041 IF (VECTOR (I,I)) 1042,1050,1060  

1042 WRITE OUTPUT TAPE 3, 1044, I, NOSTEP  

1045 GO TO 910  

1060 IF(VECTOR(I,I) - TOL) 1050,1080,1080  

1080 VAR = VECTOR(I, NOVAR) * VECTOR(NOVAR,I) / VECTOR(I,I)  

1090 IF(VAR) 1060,1170,904  

904 WRITE OUTPUT TAPE 3, 906  

   GO TO 910  

1170 VMIN = VAR  

1180 NOMIN = 1  

1190 GO TO 1050  

1190 IF (VAR - VMIN) 1050,1050,1170  

1110 IF (VAR - VMAX) 1050,1050,1210  

1220 VMAX = VAR  

1220 NUMAX = 1  

1250 CONTINUE  

1230 IF (NOIN) 903,1240,1245  

903 WRITE OUTPUT TAPE 3, 907  

   GO TO 910  

1240 WRITE OUTPUT TAPE 3,65, SIGY  

1260 GU TO 1350  

1265 IF(IFCNST) 900,1250,1246  

1266 CNS1 = 0.0  

1247 GU TO 1300

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## SUBROUTINE ESS04

(CONTINUED)

## MULTIPLE LINEAR REGRESSION CALCULATIONS

```

1250 CNST = AVE(NOVAR)           ESS04 209
1270 DO 1280 I = 1,NOIN         ESS04 210
1290 J = INDEX(I)                ESS04 211
1280 CNST = CNST - (COEN(I) * AVE(J)) ESS04 212
1300 IF (IFSTEP) 900,1310,1320    ESS04 213
1310 IF (NOIN) 1311,1311,1313    ESS04 214
1311 WRITE OUTPUT TAPE 3, 91,NOSTEP, K ESS04 215
1312 GO TO 1314                 ESS04 216
1313 WRITE OUTPUT TAPE 3, 92,NOSTEP, K ESS04 217
1314 WRITE OUTPUT TAPE 3,70,FLEVEL, SIGY,CNST, ESS04 218
   11(INDEX(J),COEN(I,J),SIGC(J),J=1,NOIN) ESS04 219
1315 GO TO NUMBER, (1320,15w0)     ESS04 220
1320 FLEVEL = VMIN + DEFR / VECTOR (NOVAR,NOVAR) ESS04 221
1330 IF(IFOUT + FLEVEL) 1330, 1350, 1340    ESS04 222
1340 K = NOIN                   ESS04 223
1345 NOIN = 0                   ESS04 224
   GO TO 1391                  ESS04 225
1350 FLEVEL = VMAX + DEFR / (VECTOR(1,NOVAR,NOVAR) - VMAX) ESS04 226
1360 IF (EFIN - FLEVEL) 1370,1361,1380    ESS04 227
1361 IF (EFIN) 1380,1380,1370    ESS04 228
1370 K = NOMAX                 ESS04 229
1390 NOIN = K                  ESS04 230
1391 IF(K) 1392,1392,1400      ESS04 231
1392 WRITE OUTPUT TAPE3, 1395, NOSTEP    ESS04 232
1394 GO TO 910                 ESS04 233
1400 DO 1410 I = 1,NOVAR        ESS04 234
1420 IF (I-K) 1430,1410,1430    ESS04 235
1430 DO 1440 J = 1, NOVAR        ESS04 236
1450 IF (J-K) 1460,1440,1460    ESS04 237
1460 VECTOR(I,J) = VECTOR(I,J) - (VECTOR(I,K) * VECTOR (K,J) / VECTOR
   - (K,K)) ESS04 238
1440 CONTINUE                  ESS04 239
1410 CONTINUE                  ESS04 240
1470 DO 1480 I = 1, NOVAR        ESS04 241
1490 IF (I-K) 1500,1480,1500    ESS04 242
1500 VECTOR (I,K) = - VECTOR (I,K) / VECTOR (K,K) ESS04 244
1480 CONTINUE                  ESS04 245
1510 DO 1520 J = 1, NOVAR        ESS04 246
1530 IF (J-K) 1540,1520,1540    ESS04 247
1540 VECTOR(K,J) = VECTOR (K,J) / VECTOR (K,K) ESS04 248
1520 CONTINUE                  ESS04 249
1550 VECTOR(K,K) = 1.0 / VECTOR(K,K) ESS04 250
1560 GO TO 1000                 ESS04 251
1380 WRITE OUTPUT TAPE 3, 75,
   9, NOSTEP                  ESS04 252
1381 IF(IFSTEP) 900,1581,1570    ESS04 254
1570 ASSIGN 1580 TO NUMBER       ESS04 255
1571 GO TO 1310                 ESS04 256
1580 GO TO 1581                 ESS04 257
1581 IFC (IPRED) 900,1582,910    ESS04 258
1582 HAVING 0                  ESS04 259
1583 WRITE OUTPUT TAPE 3, 85      ESS04 260
   CUMSUM = 0                  ESS04 261
1590 DO 1660 N = 1, NODATA      ESS04 262
1600 READ TAPE 4,(DATA(I),I= 1, NOVAR), RUN ESS04 263
1610 YPKED = CNST               ESS04 264
1620 DO 1630 I = 1,NOIN         ESS04 265
1640 K = INDEX(I)              ESS04 266
1630 YPRED= YPKED + COEN(I) * DATA(K) ESS04 267
1650 DEV = DATA(NOVAR) - YPKED ESS04 268
   CUMSUM = CUMSUM + DEV      ESS04 269
1660 WRITE OUTPUT TAPE 3,80 , RUN,DATA(NOVAR) , YPRED, DEV, CUMSUM ESS04 270
910 IF ACCUMULATOR OVERFLOW 6000,6001 ESS04 271
6001 IF QUDTINTL OVERFLOW 6000,6002 ESS04 272
6002 IF DIVIDE CHECK 6000,100 ESS04 273
6000 WRITE OUTPUT TAPE 3, 6004 ESS04 274
100 CONTINUE                  ESS04 275
   RETURN                      ESS04 276
6004 FORMAT(79HVIEW RESULTS WITH SKEPTICISM. OVERFLOW,UNDERFLOW OR DIV
   IDE CHECK HAS OCCURRED.) ESS04 277
END...
5 FORMAT (3F10.5,3I5,1H 1012) ESS04 278
6 FORMAT                           ESS04 280
  9 1H , 3F10.5 , 3I5, 1H , 1012 ) ESS04 281
10 FORMAT (6(F12.5))             ESS04 282
11 FORMAT (1H , 1PE12.5, 8E12.5 ) ESS04 283
15 FORMAT (1H 4W SUM OF VARIABLES//) ESS04 284
20 FORMAT (1H 4W SUM X(12,3H) = E12.4,8H SUM X(12,3H) =E12.4,
   18H SUM X(12,3H) =E12.4,8H SUM X(12,3H) =E12.4) ESS04 285
25 FORMAT (17H SUM Y =E12.4) ESS04 286
30 FORMAT(1H 7H RAW SUM OF SQUARES A ESS04 287
   1ND CROSS PRODUCTS// ) ESS04 288
35 FORMAT (1H 7H X(12,7H) VS X(12,3H) =E15.6, ESS04 289
   1 6H X(12,7H) VS X(12,3H) =E15.6, ESS04 290
   2 6H X(12,7H) VS X(12,3H) =E15.6, ESS04 291
40 FORMAT (1H 7H X(12,12H) VS Y =E15.6, ESS04 292
   1 6H X(12,12H) VS Y =E15.6, ESS04 293
   2 6H X(12,12H) VS Y =E15.6 ) ESS04 294
45 FORMAT (1H 21H Y VS Y =E15.6) ESS04 295
50 FORMAT (1H063H AVERAGE VALUE OF
   -VARIABLES// ) ESS04 296
55 FORMAT(1H077H RESIDUAL SUMS OF SQUA ESS04 297
   -RES AND CROSS PRODUCTS//) ESS04 298
56 FORMAT(1H069H PARTIAL CORRELATI ESS04 299
   -ON COEFFICIENTS//) ESS04 300
65 FORMAT (2SHO STANDARD ERROR OF Y = F12.6 ) ESS04 301
70 FORMAT (1H F LEVEL F12.4/2SH STANDARD ERROR OF Y = F12.4/12H ESS04 302
   1 CONSTANT E13.5/5SH VARIABLE COEFFICIENT STD ERR ESS04 303
   20 DF COEF 17H COEF/STD ERROR // (16H - X- 13) ESS04 304
   33E18.51) ESS04 305
75 FORMAT (1H COMPLETED 15,20H STEPS OF REGRESSION) ESS04 306
90 FORMAT(12H2MSTEPWISE REGRESSION //12H PROBLEM NO 110 //12H NO OF ESS04 307
   DATA = 15 //1M NO OF VARIABLES = 110 //3M WEIGHTED DEGREES OF FR ESS04 308
   21LMON = F12.2 //24H F LEVEL TO ENTER VARIABLE = F10.5 //24H F LEVE ESS04 309
   212MOM = F12.2 //24H F LEVEL TO ENTER VARIABLE = F10.5 //24H F LEVE ESS04 310
   213MOM = F12.2 //24H F LEVEL TO ENTER VARIABLE = F10.5 //24H F LEVE ESS04 311
   214MOM = F12.2 //24H F LEVEL TO ENTER VARIABLE = F10.5 //24H F LEVE ESS04 312

```

## SUBROUTINE ESS04

(CONTINUED)

## MULTIPLE LINEAR REGRESSION CALCULATIONS

31 TO REMOVE VARIABLE = F10.5 //	ESS04	313
91 FORMAT (1H0STEP NO.15 /10H VARIABLE REMOVED IS)	ESS04	314
92 FORMAT (1H0STEP NO.15 /20H VARIABLE ENTERING IS)	ESS04	315
93 FORMAT (5H RUN F10.0,3H F10.5,3H F10.5,3H F10.5, 13H F10.5,3H F10.5,3H F10.5,3H F10.5,3H F10. 25,3H F10.5,1)	ESS04	316
654 FORMAT (1H ZERO NUMBER OF DATA, SO LONG.)	ESS04	317
905 FORMAT (42H ERROR IN CONTROL CARD, PROBLEM TERMINATED)	ESS04	320
906 FORMAT (2H ERROR, VMIN PLUS, SOLONG)	ESS04	321
907 FORMAT (20H ERNOM,NOTN MINUS, SOLONG)	ESS04	322
1004 FORMAT (1H037HY SQUARE NON-POSITIVE TERMINATE STEP 1 5)	ESS04	323
1019 FORMAT (1H024H NO MORE DEGREES FREEDOM STEP 1 5 )	ESS04	324
1044 FORMAT (1H01UM SQUARE X15,17H NEGATIVE, SOLONG 15,6H STEPS)	ESS04	325
1395 FORMAT (12N RDG, STEP 16, 1H SOLONG)	ESS04	326
6112 FORMAT(1H0TOTAL CORRELATION COEFFICIENT SQUARED F10.3 )	ESS04	327
4300 FORMAT(F16.6)	ESS04	328
5003 FORMAT(1H1, 25X, 12A6 )	ESS04	329
4000 FORMAT(12A6)	ESS04	330
80 FORMAT(1X, F12.5,2X,F12.5,3X,F12.5, 2X,F12.5,2X,F12.5 )	ESS04	331
95 FORMAT(1H043H PREDICTED VS ACTUAL RESULTS /75H 1 RUN NO. ACTUAL PREDICTED DEVIATION CUMULATIV 2E SUM)	ESS04	332
5000 FORMAT( 6F12.5)	ESS04	333
END	ESS04	334
	ESS04	335
	ESS04	336

## MONSANTO RESEARCH CORPORATION FLAME SPEED REGRESSION - ROUTINE 1922 - MODIFICATION 1 - RUN 3

## MONSANTO RESEARCH CORPORATION TEST DATA FOR ROUTINE 1922

RUN 3	NUMBER OF PROBLEMS IN THIS RUN	3	HIGHEST CONTRIBUTOR CODE NUMBER IN USE	200
	ACCEPTABLE DATA SOURCE NUMBER	0	ACCEPTABLE EXPERIMENTAL CONDITIONS NUMBER	0

ENTRIES TO BE READ FROM THE INPUT DATA CARDS

CARD TYPE	NUMBER OF ENTRIES	LIST SIGNIFICANCE
-L-	0	- UNACCEPTABLE DATA GROUP SERIAL NUMBERS
-H-	0	- ACCEPTABLE FUEL CLASS NUMBERS
-M-	0	- ACCEPTABLE FUEL CLASS-GROUP NUMBERS
-G-	0	- UNACCEPTABLE FUEL-CLASS-GROUP-MEMBER NUMBERS
-P-	3	- CONTRIBUTOR COUNT TEST NUMBERS
-C-	1	- CONDITIONAL COUNT TEST CRITERIA
-R-	0	- OVERRIDING DECIMAL REGRESSION CONTROL DATA
-S-	0	- OVERRIDING INTEGER REGRESSION CONTROL DATA

## LIST OF CONTRIBUTOR COUNT TESTS

1 0 37 4 40 0

## LIST OF COUNT TEST CRITERIA

## ESSO REGRESSION CONTROL LIST

0.00100 0.00002 0.00001

1 0 1 1 1 1 0 1

## LIST OF ACCEPTED DATA SERIAL NUMBERS AND FUEL NAMES

2. ETHANE	3. PROPANE	4. NOBUTANE	5. NPENTANE	6. N-HEXANE	7. NHEPTANE
8. NOCTANE	9. N-DECANE	10. N-UNDECANE	11. N-TRIDECANE	12. ISOBUTANE	13. ISO-PENTANE
15. 22MEPENTANE	15. 2-ME-PENTANE	16. 3-ME-PENTANE	17. 23MEPENTANE	18. 22MEBUTANE	19. 24MEPENTANE
20. 23MEPENTANE	21. 224MEPENTANE	22. 225MEPENTANE	23. CYCLOPROPANE	24. CYCLOPENTENE	25. CYCLOHEXANE
26. MECYCOPENTANE	27. MECYCOPENTANE	28. 12MECYCOPENTANE	29. 12MECYCOPENTANE	30. PROPYLENE	32. BUTENE-1
33. CIS-BUTENE-2	34. TX-BUTENE-2	35. N-PENTENE-1	36. N-PENTENE-2	37. ISO-BUTYLENE	38. 3HE-BUTENE-1
39. 2-MHEUTENE-2	40. 2-MHEUTENE-2	41. 6MEPENTEN-2C	42. 6MEPENTEN-2T	43. 244MEPENTENE-1	45. 2MEBUTENE-1B
46. CYCLOHEXENE	47. 4V1-MECYCOPENTANE	48. CYCLOCIDIENE	49. PROPENE	50. 1-BUTYNE	52. TOLUENE
51. PARAXYLYLENE	56. ETHYLHENZENE	55. SECHUBENZENE	56. THIABENZENE	57. 1-F-PENTANE	58. 1-F-HEXANE
59. 1-1DIFLETHAN	60. 1-4FBUTANE	61. 11FPPENTANE	63. NE-CHLORIDE	64. ET-CHLORIDE	65. NPACHLORIDE
66. NBUCHLORIDE	67. 2BUCHLORIDE	68. 1-CLENANE	69. 1CL2MEPENTANE	70. 2CL2MEPENTANE	71. 1-4CLBUTANE
72. 1-2CLBUTANE	74. 2-CL-PROPENE	75. ALLYLCHLORIDE	76. 2CLBUTENE-2	77. ETMANOL	78. N-PROPANOL
79. ETHYLACETATE	80. 3MEBODATE	81. ME-N-AM-L-KET	82. DI-ME-ETHER	83. VI-ME-ETHER	84. P-F-ANISOLE
85. MC-WH-KETONE	86. NEAPPHKETONE	87. MEBOENAOATE	88. N-CRESOL	89. 1-3CLPROPANE	90. 1-2CLPROPANE
91. 1-BBUTANE	92. 1-2CL-ETHANE	93. 1-BB-PRHTANE	94. 2BK-BUTENE-2	95. 3-BB-PRDPENE	96. CL-22ERBANE
97. 1-2CL2FPRPAN	99. W-F-TOLUENE	101. N-BB-AMINE	112. AHE-PYRIDINE	113. ETHNDIANINE	114. 2HE-PYRIDINE
116. 1MEPABENZENE	117. 1SOPRCHLORIDE	119. 1SPRAYLBANE	120. M-BUTBENZENE	121. 124MEBENZENE	122. SECHUBENZENE
124. ORTHOXYLENE	125. METAXYLENE	126. ANISOLE	127. 1-F-PENTANE	128. 26-LUTIDINE	129. NPACHLORIDE
130. N-HEXANE	133. 1-GLPENTANE	134. 2BUTANETHIOL	135. 1-F-HEXANE	136. KTHYL3AMINE	137. DILSOPRLFOX
138. DILSOPRLFOX	139. N-BU-SULFIDE	140. ISOBURCAPTIN	142. PROPANE		

## MONSANTO RESEARCH CORPORATION FLAME SPEED REGRESSION - ROUTINE 1922 - MODIFICATION 1 - RUN 3

PROBLEM 1

-14-

DEPENDENT VARIABLE = 3 UNAX/S CHAX X10

LIST OF INDEPENDENT CONTRIBUTORS WITH THEIR CORRESPONDING REGRESSION INDICES

0 1 2 3 4 5 6 7 8 9

37 PRIM-H 38 SEC-H 39 TERI-H

1 TITLE CARD FOR ESSO REGRESSION PROGRAM  
 SIMPLE REGRESSION  
 PROBLEM NO. 1  
 NO OF DATA = 110  
 NO OF VARIABLES = 4  
 WEIGHTED DEGREES OF FREEDOM = 118.00  
 F LEVEL TO ENTER VARIABLE = 0.00002  
 F LEVEL TO REMOVE VARIABLE = 0.00001

---

STANDARD ERROR OF Y = 170.257925

STEP NO.	VARIABLE ENTERING	F LEVEL	STANDARD ERROR OF Y	CONSTANT	VARIABLE COEFFICIENT	STD ERROR OF COEF	COEF/STD ERROR	
1		315.6665	88.0189	0.	X-1	0.23660E-02	0.13200E-01	0.17773E-02

---

STEP NO. 2  
 VARIABLE ENTERING 2  
 F LEVEL 110.1560  
 STANDARD ERROR OF Y = 63.6009  
 CONSTANT 0.  
 VARIABLE COEFFICIENT STD ERROR OF COEF COEF/STD ERROR

X-1	0.18730E-02	0.10449E-01	0.17844E-02
X-2	0.12310E-02	0.11736E-01	0.10496E-02

---

STEP NO. 3  
 VARIABLE ENTERING 3  
 F LEVEL 0.5730  
 STANDARD ERROR OF Y = 63.7267  
 CONSTANT 0.  
 VARIABLE COEFFICIENT STD ERROR OF COEF COEF/STD ERROR

X-1	0.19356E-02	0.11313E-01	0.16540E-02
X-2	0.12261E-02	0.11802E-01	0.10372E-02
X-3	-0.84304E-01	0.11137E-02	-0.75695E-00

COMPLETED 3 STEPS OF REGRESSION

APPENDIX C

Fortran Programs for Routines  
FSRTL and FSRDM

## ROUTINE FSRTL

## MASTER LIBRARY TAPE PREPARATION FROM CARD LIBRARY

```

CFSRTL  MASTER TAPE PREPARATION FOR FLAME SPEED REGRESSION ROUTINE      FSRTL  1
       DIMENSION D1(6), LFGCCN(200), FSCL(200), DNHL(6)                      FSRTL  2
C   INPUT DATA FROM CARD IMAGES ON TAPE 2                                FSRTL  3
C   MASTER TAPE LOGICAL UNIT 4                                         FSRTL  4
C   REVISION 6                                                       FSRTL  5
C   TITLE CARD.                                                       FSRTL  6
C   READ INPUT TAPE 2, 1000                                              FSRTL  7
C   WRITE OUTPUT TAPE 6, 1000                                              FSRTL  8
C   NUMBER OF GROUPS ON TAPE                                           FSRTL  9
C   READ INPUT TAPE 2, 1001, IPI                                         FSRTL 10
C   WRITE OUTPUT TAPE 6,1001, IPI                                         FSRTL 11
C   MAIN DATA GROUPS                                                 FSRTL 12
C   DO 20 I=1, IPI
C     READ INPUT TAPE 2,1002, ISPN, EN1, FN2, IPNC, IPNG, IENM,
C     1 INDS, INEC, ( DIK), K=2,6), IPFGC,(LPGCCN(K), PGCL(K),K=1,
C     2 IPFGC )                                              FSRTL 14
C   20 WRITE OUTPUT TAPE 6,2002,ISPN,FN1, FN2, IPNC, IPNG, IPNM,
C     1 INDS, INEC, ( DIK), K=2,6),IPFGC,(LPGCCN(K), PGCL(K),K=1,
C     2 IPFGC )                                              FSRTL 17
C   CONTRIBUTOR NAMES                                                 FSRTL 18
C   READ INPUT TAPE 2, 1003, (GNL(I),I=1, 200)                           FSRTL 19
C   WRITE OUTPUT TAPE 6, 2003,(GNL(I),I=1, 200)                           FSRTL 20
C   DEPENDENT VARIABLES                                              FSRTL 21
C   READ INPUT TAPE 2, 1003, (DNH(I),I=1,6)                               FSRTL 22
C   WRITE OUTPUT TAPE 6, 2003, (DNH(I),I=1, 6)                            FSRTL 23
C   END FILE 6                                                       FSRTL 24
C   REWIND 6                                                       FSRTL 25
C   WRITE OUTPUT TAPE 6, 2005                                         FSRTL 26
C   CALL EXIT                                                       FSRTL 27
1000 FORMAT(1H1,1IX, 6H)                                              FSRTL 28
1001 FORMAT(1H0, 16)                                              FSRTL 29
1002 FORMAT(16, 24E, 516, 2F12.5 / 3F12.5, 16, 16, F12.5 / (16, F12.6,
16, F12.6, 1A, F12.6, 1A, F12.6))                                     FSRTL 30
1003 FORMAT(12A6)                                              FSRTL 31
2002 FORMAT(1H0, 16, 24E, 516, 1P5E12.4, 1A / (1H , 1A, E12.4, 16, E12.4,
1 , 16, E12.4, 16, E12.4, 16, E12.4 ))                                     FSRTL 32
2003 FORMAT(1H0, 9(6X,A6)/1H , 6XA6, 6XA6, 6XA6, 6XA6, 6XA6,
1 6XA6, 6XA6, 6XA6 )                                              FSRTL 33
2005 FORMAT(1H1, 25X,28HTAPE 6 PREPARATION COMPLETE )                   FSRTL 34
END                                                               FSRTL 35
                                                               FSRTL 36
                                                               FSRTL 37
                                                               FSRTL 38
                                                               FSRTL 39
                                                               FSRTL 40
                                                               FSRTL 41

```

## ROUTINE FSRDN

## MASTER CARD LIBRARY MODIFICATION

```

CFSRDN  MASTER DECK MODIFICATION FOR FLAME SPEED REGRESSION ROUTINE      FSRDN   1
C      PREPARE TAPE 16 FOR PUNCHING OF CHANGES IN MASTER TAPE          FSRDN   2
C      NOMENCLATURE                                         FSRDN   3
C      NDCPOT = NUMBER OF DATA GROUPS PREVIOUSLY ON TAPE           FSRDN   4
C      NDGCHG = NUMBER OF DATA GROUPS CURRENTLY ON TAPE           FSRDN   5
C      NDGCHG(K) = NUMBER OF DATA GROUPS ALTERED                  FSRDN   6
C      IDGCNG(K) = CODE NUMBER OF ALTERED DATA GROUPS             FSRDN   7
C      NADD = NUMBER OF DATA GROUPS ADDED TO MASTER DECK            FSRDN   8
C      ICONAM = CONTRIBUTOR NAME PUNCH SWITCH 1=PUNCH 2=INIT     FSRDN   9
C      IDPNAM = INDEPENDENT VARIABLE PUNCH SWITCH 1=PUNCH 2=INIT  FSRDN  10
DIMENSION IDGCNG(10000),LFGCCN(90),FGCL(200),DNM(16)          FSRDN  11
1, D16)
REWIND 6
C      READ INPUT CONTROL DATA
READ INPUT TAPE 2, 3000, NDCPOT, NDGCHG, ICONAM, IDPNAM      FSRDN  12
IFI NDGCHG(10, 20, 10)                                         FSRDN  13
10 READ INPUT TAPE 2, 3001, (IDGCNG(K)), K=1, NDGCHG )        FSRDN  14
C      READ TITLE AND NUMBER OF GROUPS FROM MASTER TAPE AND PUNCH    FSRDN  15
20 READ INPUT TAPE 6, 1000
READ INPUT TAPE 6, 1001, NDCPOT
WRITE OUTPUT TAPE 14, 1000
WRITE OUTPUT TAPE 3, 1000
L = 1
WRITE OUTPUT TAPE 14, 1001, NDCPOT
WRITE OUTPUT TAPE 3, 1001, NDCPOT
IFI NDCPOT = NDCPOT(100, 30, 30)                                FSRDN  23
30 DO 45 L=1, NDCPOT
READ INPUT TAPE A, 2002, ISBN, ENL, FN2, IFNC, IPNG, IFNM,      FSRDN  24
1  INDS, INEC, I (DK), K=2,61, IPFGC,(LFGCCN(K)), FGCL(K),K=1,   FSRDN  25
2  IPFGC )
3  IFI I = NDGCHG(32, 32, 36)                                 FSRDN  26
32 IFI I = NDGCHG(L, ) 40, 33, 40
33 L = L + 1
36 WRITE OUTPUT TAPE A, 2002, ISBN, ENL, FN2, IFNC, IPNG, IFNM,   FSRDN  27
1  INDS, INEC, I (DK), K=2,61, IPFGC,(LFGCCN(K)), FGCL(K),K=1,   FSRDN  28
2  IPFGC )
40 WRITE OUTPUT TAPE 3, 2002, ISPN, FN1, FN2, IFNC, IPNG, IFNM,   FSRDN  29
1  INDS, INEC, I (DK), K=2,61, IPFGC,(LFGCCN(K)), FGCL(K),K=1,   FSRDN  30
2  IPFGC )
45 CONTINUE
READ INPUT TAPE 6, 2003, (GNL(I)), I=1, 2001
READ INPUT TAPE 6, 2003, (DNM(I)), I=1, 61
GO TO (50, 60),ICONAM
50 WRITE OUTPUT TAPE 14, 1003, (GNL(I)), I=1, 2001
WRITE OUTPUT TAPE 3, 1003, (GNL(I)), I=1, 2001
60 GO TO (70, 80), IDPNAM
70 WRITE OUTPUT TAPE 14, 1003, (DNM(I)), I=1, 61
WRITE OUTPUT TAPE 3, 1003, (DNM(I)), I=1, 61
80 WRITE OUTPUT TAPE 3, 4000
90 CALL EXIT
100 WRITE OUTPUT TAPE 3, 4001
GO TO 90
1000 FORMAT(1H1,11X,-60H)
1
1001 FORMAT(1H0, -1A1)
1002 FORMAT(16, 2A6, 5I6, 2E12.5 / 3E12.5, 16, 16, E12.5 / 16, E12.5,
1  16, E12.5,-16, E12.5,-16,E12.5)
1003 FORMAT(12A6)
2002 FORMAT(1H0, 16, 2A6, 5I6, 1P5E12.4, 16, 1H,-16, E12.4, 16, E12.4
1, 16, E12.4, 16, E12.4, 16, E12.4, 16, E12.4 )
2003 FORMAT(1H0, -9AX, A6Z2/1H , AXAA, AXAA, AXAA, AXAA, AXAA, AXAA)
3000 FORMAT( 4I6)
3001 FORMAT( 12I6)
4000 FORMAT(1H1, 25X, 35HMASTER DECK MODIFICATION COMPLETE)
4001 FORMAT(1H1, 25X, 48MERROR - MORE DATA GROUPS IN LIBRARY THAN ON TAP
IE )
END

```

